Pentadecylbenzene

Other names:	1-phenylpentadecane
	benzene, pentadecyl-
	n-pentadecylbenzene
	pentadecane, 1-phenyl-
Inchi:	InChI=1S/C21H36/c1-2-3-4-5-6-7-8-9-10-11-12-13-15-18-21-19-16-14-17-20-21/h14,16-1
InchiKey:	JIRNEODMTPGRGV-UHFFFAOYSA-N
Formula:	C21H36
SMILES:	CCCCCCCCCCCCCCCc1ccccc1
Mol. weight [g/mol]:	288.52
CAS:	2131-18-2

Physical Properties

Property code	Value	Unit	Source
af	0.8501		Cheméo Relay (1.0)
gf	238.35	kJ/mol	Joback Method
hf	-225.81	kJ/mol	Cheméo Relay (1.0)
hfus	44.19	kJ/mol	Joback Method
hvap	102.27	kJ/mol	Cheméo Relay (1.0)
ie	9.07	eV	Cheméo Relay (1.0)
log10ws	-8.01		Cheméo Relay (1.0)
logp	7.320		Crippen Method
mcvol	282.990	ml/mol	McGowan Method
pc	1186.60	kPa	Joback Method
tb	613.18	K	Cheméo Relay (1.0)
tc	794.96	K	Cheméo Relay (1.0)
tf	288.98	K	Cheméo Relay (1.0)
vc	1.114	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	825.61	J/mol×K	706.56	Joback Method
cpg	933.63	J/mol×K	889.03	Joback Method
cpg	917.95	J/mol×K	858.62	Joback Method

cpg	901.40	J/mol×K	828.21	Joback Method
cpg	883.93	J/mol×K	797.79	Joback Method
cpg	865.51	J/mol×K	767.38	Joback Method
cpg	846.08	J/mol×K	736.97	Joback Method
dvisc	0.0002591	Pa×s	529.70	Joback Method
dvisc	0.0000865	Pa×s	706.56	Joback Method
dvisc	0.0001167	Pa×s	647.61	Joback Method
dvisc	0.0001671	Pa×s	588.66	Joback Method
dvisc	0.0023303	Pa×s	352.85	Joback Method
dvisc	0.0004486	Pa×s	470.75	Joback Method
dvisc	0.0009087	Pa×s	411.80	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tfp	285.10	K	100.00	Solid-Liquid Equilibria under High Pressure of Nine Pure n-Alkylbenzenes
tfp	289.70	K	21000.00	Solid-Liquid Equilibria under High Pressure of Nine Pure n-Alkylbenzenes
tfp	294.10	K	40100.00	Solid-Liquid Equilibria under High Pressure of Nine Pure n-Alkylbenzenes
tfp	298.40	K	59900.00	Solid-Liquid Equilibria under High Pressure of Nine Pure n-Alkylbenzenes
tfp	302.80	K	80400.00	Solid-Liquid Equilibria under High Pressure of Nine Pure n-Alkylbenzenes
tfp	306.70	K	100200.00	Solid-Liquid Equilibria under High Pressure of Nine Pure n-Alkylbenzenes

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.59172e+01
Coeff. B	-6.09906e+03
Coeff. C	-9.90840e+01
Temperature range (K), min.	489.31
Temperature range (K), max.	674.16

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2131182&Units=SI
Cheméo Relay (1.0, beta):	
Solid-Liquid Equilibria under High Pressure of Nine Pure n-Alkylbenzenes:	https://www.doi.org/10.1021/je700529y
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Cheméo Relay (1.0):	

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tfp:	Melting point
vc:	Critical Volume