Benzene, (1-hexyltetradecyl)-

Other names:	Eicosane, 7-phenyl-
	7-Phenyleicosane
Inchi:	InChI=1S/C26H46/c1-3-5-7-9-10-11-12-13-14-15-18-22-25(21-17-8-6-4-2)26-23-19-16-2
InchiKey:	DGROBZZOOZUCTC-UHFFFAOYSA-N
Formula:	C26H46
SMILES:	CCCCCCCCCCCCCC(CCCCCC)c1ccccc1
Mol. weight [g/mol]:	358.64
CAS:	2398-64-3

Physical Properties

Property code	Value	Unit	Source
gf	278.01	kJ/mol	Joback Method
hf	-348.72	kJ/mol	Joback Method
hfus	53.61	kJ/mol	Joback Method
hvap	75.36	kJ/mol	Joback Method
ie	9.00 ± 0.10	eV	NIST Webbook
log10ws	-9.77		Crippen Method
logp	9.442		Crippen Method
mcvol	353.440	ml/mol	McGowan Method
pc	877.91	kPa	Joback Method
tb	820.52	K	Joback Method
tc	1009.19	K	Joback Method
tf	394.20	K	Joback Method
vc	1.377	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1247.45	J/mol×K	1009.19	Joback Method
cpg	1230.90	J/mol×K	977.74	Joback Method
cpg	1213.40	J/mol×K	946.30	Joback Method
cpg	1194.89	J/mol×K	914.85	Joback Method
cpg	1175.33	J/mol×K	883.41	Joback Method
cpg	1154.64	J/mol×K	851.96	Joback Method

cpg	1132.76	J/mol×K	820.52	Joback Method
dvisc	0.0017071	Pa×s	394.20	Joback Method
dvisc	0.0000410	Pa×s	820.52	Joback Method
dvisc	0.0000568	Pa×s	749.47	Joback Method
dvisc	0.0000844	Pa×s	678.41	Joback Method
dvisc	0.0001374	Pa×s	607.36	Joback Method
dvisc	0.0002548	Pa×s	536.31	Joback Method
dvisc	0.0005703	Pa×s	465.25	Joback Method
hvapt	93.80	kJ/mol	501.50	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2398643&Units=SI

Legend

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
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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