2-Phenyleicosane

Other names: Eicosane, 2-phenyl-
2-Phenyleicosane
Inchi: InChI=1S/C26H46/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-19-22-25(2)26-23-20-18-21
InchiKey: GWTSUVHHMPSJLJ-UHFFFAOYSA-N
Formula: C26H46
SMILES: CCCCCCCCCCCCCCCCCCC(C)c1ccccc1
Mol. weight [g/mol]: 358.65

Physical Properties

Property code	Value	Unit	Source
af	0.9666		Cheméo Relay (1.0)
gf	278.01	kJ/mol	Joback Method
hf	-352.66	kJ/mol	Cheméo Relay (1.0)
hfus	53.61	kJ/mol	Joback Method
hvap	122.29	kJ/mol	Cheméo Relay (1.0)
ie	9.20 ± 0.10	eV	NIST Webbook
log10ws	-9.27		Cheméo Relay (1.0)
logp	9.442		Crippen Method
mcvol	353.440	ml/mol	McGowan Method
pc	877.91	kPa	Joback Method
tb	635.87	K	Cheméo Relay (1.0)
tc	831.15	K	Cheméo Relay (1.0)
tf	299.44	K	Cheméo Relay (1.0)
vc	1.362	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

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

cpg	1132.76	J/mol×K	820.52	Joback Method
dvisc	0.0002548	Pa×s	536.31	Joback Method
dvisc	0.0005703	Pa×s	465.25	Joback Method
dvisc	0.0017071	Pa×s	394.20	Joback Method
dvisc	0.0001374	Pa×s	607.36	Joback Method
dvisc	0.0000844	Pa×s	678.41	Joback Method
dvisc	0.0000568	Pa×s	749.47	Joback Method
dvisc	0.0000410	Pa×s	820.52	Joback Method
hvapt	90.40	kJ/mol	511.50	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2398665&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
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