

Benzene, (1-butylhexadecyl)-

Other names:	Eicosane, 5-phenyl- 5-Phenyleicosane
Inchi:	InChI=1S/C26H46/c1-3-5-7-8-9-10-11-12-13-14-15-16-18-22-25(21-6-4-2)26-23-19-17-20
InchiKey:	KINRJYWUZLHOKP-UHFFFAOYSA-N
Formula:	C26H46
SMILES:	CCCCCCCCCCCCCCCC(CCCC)c1ccccc1
Mol. weight [g/mol]:	358.64
CAS:	2400-04-6

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
mvol	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	267.00 ± 4.00	K	NIST Webbook
vc	1.377	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1247.45	J/mol×K	1009.19	Joback Method
cpg	1132.76	J/mol×K	820.52	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	1230.90	J/molxK	977.74	Joback Method
dvisc	0.0000410	Paxs	820.52	Joback Method
dvisc	0.0017071	Paxs	394.20	Joback Method
dvisc	0.0005703	Paxs	465.25	Joback Method
dvisc	0.0002548	Paxs	536.31	Joback Method
dvisc	0.0001374	Paxs	607.36	Joback Method
dvisc	0.0000844	Paxs	678.41	Joback Method
dvisc	0.0000568	Paxs	749.47	Joback Method
hvapt	94.30	kJ/mol	503.00	NIST Webbook

Sources

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=C2400046&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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