

Benzene, 1,4-dihexadecyl-

Inchi:	InChI=1S/C38H70/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-31-37-33-35-38(36-34-37)
InchiKey:	IDQPYQHFNWSAFI-UHFFFAOYSA-N
Formula:	C38H70
SMILES:	CCCCCCCCCCCCCCCCc1ccc(CCCCCCCCCCCCCCCC)cc1
Mol. weight [g/mol]:	526.96
CAS:	55517-88-9

Physical Properties

Property code	Value	Unit	Source
gf	371.86	kJ/mol	Joback Method
hf	-602.59	kJ/mol	Joback Method
hfus	87.83	kJ/mol	Joback Method
hvap	103.12	kJ/mol	Joback Method
log10ws	-14.80		Crippen Method
logp	13.734		Crippen Method
mcvol	522.520	ml/mol	McGowan Method
pc	483.03	kPa	Joback Method
tb	1100.50	K	Joback Method
tc	1399.25	K	Joback Method
tf	556.96	K	Joback Method
vc	2.055	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1930.68	J/molxK	1100.50	Joback Method
cpg	2068.05	J/molxK	1349.45	Joback Method
cpg	2044.06	J/molxK	1299.66	Joback Method
cpg	2018.66	J/molxK	1249.87	Joback Method
cpg	1991.51	J/molxK	1200.08	Joback Method
cpg	1962.29	J/molxK	1150.29	Joback Method
cpg	2090.95	J/molxK	1399.25	Joback Method
dvisc	0.0000074	Paxs	1100.50	Joback Method
dvisc	0.0000102	Paxs	1009.91	Joback Method

dvisc	0.0000149	Paxs	919.32	Joback Method
dvisc	0.0000236	Paxs	828.73	Joback Method
dvisc	0.0000418	Paxs	738.14	Joback Method
dvisc	0.0000870	Paxs	647.55	Joback Method
dvisc	0.0002301	Paxs	556.96	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C55517889&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
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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