

Methylamine, N,N-bis(n.-hexadecyl)-

Other names:	1-Hexadecanamine, N-hexadecyl-N-methyl-
Inchi:	InChI=1S/C33H69N/c1-4-6-8-10-12-14-16-18-20-22-24-26-28-30-32-34(3)33-31-29-27-2
InchiKey:	KCMTVIZYKDBFFS-UHFFFAOYSA-N
Formula:	C33H69N
SMILES:	CCCCCCCCCCCCCCCCCN(C)CCCCCCCCCCCCCCCCC
Mol. weight [g/mol]:	479.92

Physical Properties

Property code	Value	Unit	Source
af	1.3204		Cheméo Relay (1.0)
gf	337.76	kJ/mol	Joback Method
hf	-674.16	kJ/mol	Cheméo Relay (1.0)
hfus	84.25	kJ/mol	Joback Method
hvap	156.51	kJ/mol	Cheméo Relay (1.0)
ie	8.63	eV	Cheméo Relay (1.0)
log10ws	-10.43		Cheméo Relay (1.0)
logp	11.881		Crippen Method
mcvol	485.810	ml/mol	McGowan Method
pc	519.36	kPa	Joback Method
tb	670.83	K	Cheméo Relay (1.0)
tc	833.83	K	Cheméo Relay (1.0)
tf	307.65 ± 2.00	K	NIST Webbook
vc	1.916	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1734.27	J/mol×K	966.88	Joback Method
cpg	1765.93	J/mol×K	1008.14	Joback Method
cpg	1795.50	J/mol×K	1049.40	Joback Method
cpg	1823.14	J/mol×K	1090.66	Joback Method
cpg	1849.04	J/mol×K	1131.92	Joback Method
cpg	1873.36	J/mol×K	1173.18	Joback Method
cpg	1896.28	J/mol×K	1214.43	Joback Method

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=C16724611&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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