

Octacosylamine, N,N-dimethyl-

Inchi: InChI=1S/C30H63N/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25-26-27-28-29-30
InchiKey: JWZUMFXLRAZKDS-UHFFFAOYSA-N
Formula: C30H63N
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCN(C)C
Mol. weight [g/mol]: 437.83

Physical Properties

Property code	Value	Unit	Source
gf	312.50	kJ/mol	Joback Method
hf	-595.00	kJ/mol	Joback Method
hfus	76.48	kJ/mol	Joback Method
hvap	84.42	kJ/mol	Joback Method
log10ws	-10.95		Crippen Method
logp	10.710		Crippen Method
mvol	443.540	ml/mol	McGowan Method
pc	594.88	kPa	Joback Method
rinpol	3109.00		NIST Webbook
tb	898.24	K	Joback Method
tc	1109.98	K	Joback Method
tf	460.33	K	Joback Method
vc	1.734	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1528.99	J/molxK	898.24	Joback Method
cpg	1556.87	J/molxK	933.53	Joback Method
cpg	1583.14	J/molxK	968.82	Joback Method
cpg	1607.90	J/molxK	1004.11	Joback Method
cpg	1631.24	J/molxK	1039.40	Joback Method
cpg	1653.28	J/molxK	1074.69	Joback Method
cpg	1674.11	J/molxK	1109.98	Joback Method

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=U406309&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

Legend

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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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