Distearyl methyl amine

Other names: N-methyldioctadecylamine
Inchi: InChI=1S/C37H77N/c1-4-6-8-10-12-14-16-18-20-22-24-26-28-30-32-34-36-38(3)37-35-3
InchiKey: VFLWKHBYVIUAMP-UHFFFAOYSA-N
Formula: C37H77N
SMILES: CCCCCCCCCCCCCCCCCCN(C)CCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 536.01
CAS: 4088-22-6

Physical Properties

Property code	Value	Unit	Source
gf	371.44	kJ/mol	Joback Method
hf	-739.48	kJ/mol	Joback Method
hfus	94.61	kJ/mol	Joback Method
hvap	100.00	kJ/mol	Joback Method
log10ws	-13.88		Crippen Method
logp	13.441		Crippen Method
mcvol	542.170	ml/mol	McGowan Method
pc	439.14	kPa	Joback Method
rinpol	3700.00		NIST Webbook
rinpol	3700.00		NIST Webbook
tb	1058.40	K	Joback Method
tc	1376.85	K	Joback Method
tf	313.15 ± 2.00	K	NIST Webbook
vc	2.126	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2012.92	J/mol×K	1058.40	Joback Method
cpg	2051.68	J/mol×K	1111.47	Joback Method
cpg	2087.36	J/mol×K	1164.55	Joback Method
cpg	2120.38	J/mol×K	1217.62	Joback Method
cpg	2151.16	J/mol×K	1270.70	Joback Method
cpg	2180.12	J/mol×K	1323.77	Joback Method

cpg	2207.68	J/mol×K	1376.85	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.54294e+01
Coeff. B	-6.79116e+03
Coeff. C	-1.58254e+02
Temperature range (K), min.	606.76
Temperature range (K), max.	829.46

Sources

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=C4088226&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices

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