N-[3-(dimethylamino)propyl]octadecanamide

Other names: N-[3-(dimethylamino)propyl]stearamide
Inchi: InChI=1S/C23H48N2O/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-20-23(26)24-21-19-2
InchiKey: WWVIUVHFPSALDO-UHFFFAOYSA-N
Formula: C23H48N2O
SMILES: CCCCCCCCCCCCCCCCCC(=O)NCCCN(C)C
Mol. weight [g/mol]: 368.64
CAS: 7651-02-7

Physical Properties

Property code	Value	Unit	Source
gf	214.03	kJ/mol	Joback Method
hf	-509.63	kJ/mol	Joback Method
hfus	65.05	kJ/mol	Joback Method
hvap	82.02	kJ/mol	Joback Method
log10ws	-6.98		Crippen Method
logp	6.316		Crippen Method
mcvol	356.460	ml/mol	McGowan Method
pc	890.00	kPa	Joback Method
tb	842.12	K	Joback Method
tc	1031.00	K	Joback Method
tf	484.03	K	Joback Method
vc	1.383	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1174.14	J/mol×K	842.12	Joback Method
cpg	1195.42	J/mol×K	873.60	Joback Method
cpg	1215.55	J/mol×K	905.08	Joback Method
cpg	1234.59	J/mol×K	936.56	Joback Method
cpg	1252.59	J/mol×K	968.04	Joback Method
cpg	1269.61	J/mol×K	999.52	Joback Method
cpg	1285.71	J/mol×K	1031.00	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=C7651027&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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