Pentadecanoic acid, 2-(dimethylamino)ethyl ester

Inchi: InChI=1S/C19H39NO2/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-19(21)22-18-17-20(2)3/h4-1

InchiKey: YDAFEAGUDJFURU-UHFFFAOYSA-N

Formula: C19H39NO2

SMILES: CCCCCCCCCCCCCCC(=O)OCCN(C)C

Mol. weight [g/mol]: 313.52

Physical Properties

Property code	Value	Unit	Source
gf	-14.04	kJ/mol	Joback Method
hf	-612.76	kJ/mol	Joback Method
hfus	50.77	kJ/mol	Joback Method
hvap	69.09	kJ/mol	Joback Method
log10ws	-5.21		Crippen Method
logp	5.182		Crippen Method
mcvol	295.990	ml/mol	McGowan Method
pc	1112.59	kPa	Joback Method
tb	722.85	K	Joback Method
tc	892.87	K	Joback Method
tf	408.52	K	Joback Method
vc	1.141	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	891.44	J/mol×K	722.85	Joback Method
cpg	910.86	J/mol×K	751.19	Joback Method
cpg	929.37	J/mol×K	779.52	Joback Method
cpg	947.00	J/mol×K	807.86	Joback Method
cpg	963.76	J/mol×K	836.20	Joback Method
cpg	979.69	J/mol×K	864.53	Joback Method
cpg	994.81	J/mol×K	892.87	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=B6008061&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