Sarcosine, N-isobutyryl-, octadecyl ester

Inchi: InChI=1S/C25H49NO3/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-29-24(27)22-
InchiKey: RYVNABYWBZYPEW-UHFFFAOYSA-N
Formula: C25H49NO3
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)CN(C)C(=O)C(C)C
Mol. weight [g/mol]: 411.66

Physical Properties

Property code	Value	Unit	Source
gf	-94.88	kJ/mol	Joback Method
hf	-854.46	kJ/mol	Joback Method
hfus	64.39	kJ/mol	Joback Method
hvap	88.80	kJ/mol	Joback Method
log10ws	-7.25		Crippen Method
logp	6.905		Crippen Method
mcvol	382.100	ml/mol	McGowan Method
pc	814.93	kPa	Joback Method
rinpol	3074.00		NIST Webbook
rinpol	3074.00		NIST Webbook
tb	913.56	K	Joback Method
tc	1120.67	K	Joback Method
tf	511.07	K	Joback Method
vc	1.478	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1293.82	J/mol×K	913.56	Joback Method
cpg	1315.00	J/mol×K	948.08	Joback Method
cpg	1334.76	J/mol×K	982.60	Joback Method
cpg	1353.17	J/mol×K	1017.12	Joback Method
cpg	1370.30	J/mol×K	1051.63	Joback Method
cpg	1386.21	J/mol×K	1086.15	Joback Method
cpg	1400.95	J/mol×K	1120.67	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321279&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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
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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