Sarcosine, N-isobutyryl-, heptadecyl ester

Inchi: InChI=1S/C24H47NO3/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-28-23(26)21-25(
InchiKey: LRJWHJIDSPAQFU-UHFFFAOYSA-N
Formula: C24H47NO3
SMILES: CCCCCCCCCCCCCCCCCOC(=O)CN(C)C(=O)C(C)C
Mol. weight [g/mol]: 397.63

Physical Properties

Property code	Value	Unit	Source
gf	-103.30	kJ/mol	Joback Method
hf	-833.82	kJ/mol	Joback Method
hfus	61.80	kJ/mol	Joback Method
hvap	86.58	kJ/mol	Joback Method
log10ws	-6.83		Crippen Method
logp	6.515		Crippen Method
mcvol	368.010	ml/mol	McGowan Method
pc	861.50	kPa	Joback Method
rinpol	2917.00		NIST Webbook
rinpol	2917.00		NIST Webbook
tb	890.68	K	Joback Method
tc	1091.05	K	Joback Method
tf	499.80	K	Joback Method
vc	1.421	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1230.02	J/mol×K	890.68	Joback Method
cpg	1250.61	J/mol×K	924.07	Joback Method
cpg	1269.89	J/mol×K	957.47	Joback Method
cpg	1287.90	J/mol×K	990.86	Joback Method
cpg	1304.71	J/mol×K	1024.26	Joback Method
cpg	1320.37	J/mol×K	1057.65	Joback Method
cpg	1334.93	J/mol×K	1091.05	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=U321278&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
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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