Sarcosine, N-isobutyryl-, hexadecyl ester

Inchi: InChI=1S/C23H45NO3/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-27-22(25)20-24(4)2
InchiKey: RXGNTFSQIFMBOR-UHFFFAOYSA-N
Formula: C23H45NO3
SMILES: CCCCCCCCCCCCCCCCOC(=O)CN(C)C(=O)C(C)C
Mol. weight [g/mol]: 383.61

Physical Properties

Property code	Value	Unit	Source
gf	-111.72	kJ/mol	Joback Method
hf	-813.18	kJ/mol	Joback Method
hfus	59.21	kJ/mol	Joback Method
hvap	84.35	kJ/mol	Joback Method
log10ws	-6.42		Crippen Method
logp	6.125		Crippen Method
mcvol	353.920	ml/mol	McGowan Method
pc	912.18	kPa	Joback Method
rinpol	2787.00		NIST Webbook
rinpol	2787.00		NIST Webbook
tb	867.80	K	Joback Method
tc	1062.44	K	Joback Method
tf	488.53	K	Joback Method
vc	1.365	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1166.79	J/mol×K	867.80	Joback Method
cpg	1186.85	J/mol×K	900.24	Joback Method
cpg	1205.67	J/mol×K	932.68	Joback Method
cpg	1223.32	J/mol×K	965.12	Joback Method
cpg	1239.83	J/mol×K	997.56	Joback Method
cpg	1255.25	J/mol×K	1030.00	Joback Method
cpg	1269.63	J/mol×K	1062.44	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321277&Units=SI

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