Sarcosine, N-isobutyryl-, tetradecyl ester

Inchi: InChI=1S/C21H41NO3/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-25-20(23)18-22(4)21(24)1
InchiKey: XSPARGVZEQSIPS-UHFFFAOYSA-N
Formula: C21H41NO3
SMILES: CCCCCCCCCCCCCCOC(=O)CN(C)C(=O)C(C)C
Mol. weight [g/mol]: 355.56

Physical Properties

Property code	Value	Unit	Source
gf	-128.56	kJ/mol	Joback Method
hf	-771.90	kJ/mol	Joback Method
hfus	54.03	kJ/mol	Joback Method
hvap	79.90	kJ/mol	Joback Method
log10ws	-5.58		Crippen Method
logp	5.345		Crippen Method
mcvol	325.740	ml/mol	McGowan Method
pc	1027.94	kPa	Joback Method
rinpol	2567.00		NIST Webbook
rinpol	2567.00		NIST Webbook
tb	822.04	K	Joback Method
tc	1007.95	K	Joback Method
tf	465.99	K	Joback Method
vc	1.254	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1042.26	J/mol×K	822.04	Joback Method
cpg	1061.38	J/mol×K	853.03	Joback Method
cpg	1079.41	J/mol×K	884.01	Joback Method
cpg	1096.39	J/mol×K	915.00	Joback Method
cpg	1112.35	J/mol×K	945.98	Joback Method
cpg	1127.32	J/mol×K	976.97	Joback Method
cpg	1141.36	J/mol×K	1007.95	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321275&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

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