Sarcosine, N-isobutyryl-, pentadecyl ester

Inchi: InChI=1S/C22H43NO3/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-26-21(24)19-23(4)22(2
InchiKey: QAHJGYDUMHZQBG-UHFFFAOYSA-N
Formula: C22H43NO3
SMILES: CCCCCCCCCCCCCCCOC(=O)CN(C)C(=O)C(C)C
Mol. weight [g/mol]: 369.58

Physical Properties

Property code	Value	Unit	Source
gf	-120.14	kJ/mol	Joback Method
hf	-792.54	kJ/mol	Joback Method
hfus	56.62	kJ/mol	Joback Method
hvap	82.12	kJ/mol	Joback Method
log10ws	-6.00		Crippen Method
logp	5.735		Crippen Method
mcvol	339.830	ml/mol	McGowan Method
pc	967.47	kPa	Joback Method
rinpol	2673.00		NIST Webbook
tb	844.92	K	Joback Method
tc	1034.76	K	Joback Method
tf	477.26	K	Joback Method
vc	1.310	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1104.19	J/mol×K	844.92	Joback Method
cpg	1123.75	J/mol×K	876.56	Joback Method
cpg	1142.17	J/mol×K	908.20	Joback Method
cpg	1159.47	J/mol×K	939.84	Joback Method
cpg	1175.69	J/mol×K	971.48	Joback Method
cpg	1190.89	J/mol×K	1003.12	Joback Method
cpg	1205.10	J/mol×K	1034.76	Joback Method

Sources

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=U321276&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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