

Sarcosine, N-(3-methylbut-2-enoyl)-, pentadecyl ester

Inchi: InChI=1S/C23H43NO3/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-27-23(26)20-24(4)22(2)
InchiKey: SBNSQIHUFNNCE-UHFFFAOYSA-N
Formula: C23H43NO3
SMILES: CCCCCCCCCCCCCCOC(=O)CN(C)C(=O)C=C(C)C
Mol. weight [g/mol]: 381.59

Physical Properties

Property code	Value	Unit	Source
gf	-37.61	kJ/mol	Joback Method
hf	-700.47	kJ/mol	Joback Method
hfus	61.62	kJ/mol	Joback Method
hvap	84.77	kJ/mol	Joback Method
log10ws	-6.51		Crippen Method
logp	6.045		Crippen Method
mcvol	349.620	ml/mol	McGowan Method
pc	939.79	kPa	Joback Method
rinpol	2832.00		NIST Webbook
tb	872.28	K	Joback Method
tc	1068.01	K	Joback Method
tf	484.49	K	Joback Method
vc	1.353	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1139.57	J/mol×K	872.28	Joback Method
cpg	1159.05	J/mol×K	904.90	Joback Method
cpg	1177.40	J/mol×K	937.52	Joback Method
cpg	1194.69	J/mol×K	970.14	Joback Method
cpg	1210.98	J/mol×K	1002.76	Joback Method
cpg	1226.31	J/mol×K	1035.38	Joback Method
cpg	1240.75	J/mol×K	1068.01	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=U321525&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

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