

Sarcosine, N-valeryl-, decyl ester

Inchi:	InChI=1S/C18H35NO3/c1-4-6-8-9-10-11-12-13-15-22-18(21)16-19(3)17(20)14-7-5-2/h4-
InchiKey:	OMPLAPKHQUVQAX-UHFFFAOYSA-N
Formula:	C18H35NO3
SMILES:	CCCCCCCCCOC(=O)CN(C)C(=O)CCCC
Mol. weight [g/mol]:	313.48

Physical Properties

Property code	Value	Unit	Source
gf	-151.38	kJ/mol	Joback Method
hf	-704.70	kJ/mol	Joback Method
hfus	49.78	kJ/mol	Joback Method
hvap	73.61	kJ/mol	Joback Method
log10ws	-4.56		Crippen Method
logp	4.319		Crippen Method
mcvol	283.470	ml/mol	McGowan Method
pc	1240.71	kPa	Joback Method
rinpola	2313.00		NIST Webbook
tb	753.84	K	Joback Method
tc	931.11	K	Joback Method
tf	447.18	K	Joback Method
vc	1.091	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	860.75	J/mol×K	753.84	Joback Method
cpg	878.53	J/mol×K	783.38	Joback Method
cpg	895.40	J/mol×K	812.93	Joback Method
cpg	911.37	J/mol×K	842.47	Joback Method
cpg	926.47	J/mol×K	872.02	Joback Method
cpg	940.74	J/mol×K	901.56	Joback Method
cpg	954.19	J/mol×K	931.11	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=U321565&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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	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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