

Sarcosine, n-pentafluorobenzoyl-, pentadecyl ester

Inchi:	InChI=1S/C25H36F5NO3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-34-18(32)17-31(2)25(3
InchiKey:	CEOWCCZAKHOTFS-UHFFFAOYSA-N
Formula:	C25H36F5NO3
SMILES:	CCCCCCCCCCCCCOC(=O)CN(C)C(=O)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]:	493.55

Physical Properties

Property code	Value	Unit	Source
gf	-1002.23	kJ/mol	Joback Method
hf	-1650.55	kJ/mol	Joback Method
hfus	75.41	kJ/mol	Joback Method
hvap	90.69	kJ/mol	Joback Method
log10ws	-8.83		Crippen Method
logp	7.089		Crippen Method
mcvol	367.190	ml/mol	McGowan Method
pc	825.74	kPa	Joback Method
rinsol	2896.00		NIST Webbook
tb	961.93	K	Joback Method
tc	1187.02	K	Joback Method
tf	618.04	K	Joback Method
vc	1.466	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1227.42	J/molxK	961.93	Joback Method
cpg	1245.05	J/molxK	999.44	Joback Method
cpg	1261.16	J/molxK	1036.96	Joback Method
cpg	1275.80	J/molxK	1074.47	Joback Method
cpg	1289.05	J/molxK	1111.99	Joback Method
cpg	1300.95	J/molxK	1149.50	Joback Method
cpg	1311.56	J/molxK	1187.02	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321555&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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