

Sarcosine, N-(3-fluorobenzoyl)-, pentadecyl ester

Inchi: InChI=1S/C25H40FNO3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-19-30-24(28)21-27(2)25(29)
InchiKey: KATLLCTYWBNWOV-UHFFFAOYSA-N
Formula: C25H40FNO3
SMILES: CCCCCCCCCCCCCCOC(=O)CN(C)C(=O)c1cccc(F)c1
Mol. weight [g/mol]: 421.59

Physical Properties

Property code	Value	Unit	Source
gf	-184.47	kJ/mol	Joback Method
hf	-820.23	kJ/mol	Joback Method
hfus	64.64	kJ/mol	Joback Method
hvap	91.31	kJ/mol	Joback Method
log10ws	-7.51		Crippen Method
logp	6.532		Crippen Method
mcvol	360.110	ml/mol	McGowan Method
pc	952.60	kPa	Joback Method
tb	944.93	K	Joback Method
tc	1157.04	K	Joback Method
tf	565.60	K	Joback Method
vc	1.393	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1201.92	J/mol×K	944.93	Joback Method
cpg	1219.78	J/mol×K	980.28	Joback Method
cpg	1236.34	J/mol×K	1015.63	Joback Method
cpg	1251.65	J/mol×K	1050.99	Joback Method
cpg	1265.78	J/mol×K	1086.34	Joback Method
cpg	1278.81	J/mol×K	1121.69	Joback Method
cpg	1290.79	J/mol×K	1157.04	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321396&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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