

Sarcosine, N-(2,6-difluorobenzoyl)-, tetradecyl ester

Inchi:	InChI=1S/C24H37F2NO3/c1-3-4-5-6-7-8-9-10-11-12-13-14-18-30-22(28)19-27(2)24(29)2
InchiKey:	MQEAJCBADXATGL-UHFFFAOYSA-N
Formula:	C24H37F2NO3
SMILES:	CCCCCCCCCCCCCCCCOC(=O)CN(C)C(=O)c1c(F)cccc1F
Mol. weight [g/mol]:	425.55

Physical Properties

Property code	Value	Unit	Source
gf	-397.33	kJ/mol	Joback Method
hf	-1007.17	kJ/mol	Joback Method
hfus	64.75	kJ/mol	Joback Method
hvap	88.93	kJ/mol	Joback Method
log10ws	-7.42		Crippen Method
logp	6.281		Crippen Method
mcvol	347.790	ml/mol	McGowan Method
pc	974.13	kPa	Joback Method
tb	926.30	K	Joback Method
tc	1134.18	K	Joback Method
tf	567.44	K	Joback Method
vc	1.355	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1146.40	J/mol×K	926.30	Joback Method
cpg	1163.66	J/mol×K	960.95	Joback Method
cpg	1179.67	J/mol×K	995.59	Joback Method
cpg	1194.47	J/mol×K	1030.24	Joback Method
cpg	1208.12	J/mol×K	1064.89	Joback Method
cpg	1220.68	J/mol×K	1099.53	Joback Method
cpg	1232.21	J/mol×K	1134.18	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=U321303&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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