

Sarcosine, n-pentafluorobenzoyl-, decyl ester

Inchi:	InChI=1S/C20H26F5NO3/c1-3-4-5-6-7-8-9-10-11-29-13(27)12-26(2)20(28)14-15(21)17(2)
InchiKey:	ROFWNDNAIDISIR-UHFFFAOYSA-N
Formula:	C20H26F5NO3
SMILES:	CCCCCCCCCOC(=O)CN(C)C(=O)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]:	423.42

Physical Properties

Property code	Value	Unit	Source
gf	-1044.33	kJ/mol	Joback Method
hf	-1547.35	kJ/mol	Joback Method
hfus	62.46	kJ/mol	Joback Method
hvap	79.56	kJ/mol	Joback Method
log10ws	-6.74		Crippen Method
logp	5.138		Crippen Method
mvol	296.740	ml/mol	McGowan Method
pc	1111.11	kPa	Joback Method
rinpol	2363.00		NIST Webbook
rinpol	2363.00		NIST Webbook
tb	847.53	K	Joback Method
tc	1037.87	K	Joback Method
tf	561.69	K	Joback Method
vc	1.185	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	924.83	J/mol×K	847.53	Joback Method
cpg	939.66	J/mol×K	879.25	Joback Method
cpg	953.52	J/mol×K	910.98	Joback Method
cpg	966.41	J/mol×K	942.70	Joback Method
cpg	978.37	J/mol×K	974.43	Joback Method
cpg	989.41	J/mol×K	1006.15	Joback Method
cpg	999.56	J/mol×K	1037.87	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=U321551&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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