

Benzamide, 2,5-difluoro-N-(2,5-difluorobenzoyl)-N-tetradecyl-

Inchi: InChI=1S/C28H35F4NO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-18-33(27(34)23-19-21(29)14-15-16-17)/N
InchiKey: FJGUTTKIYPTKMI-UHFFFAOYSA-N
Formula: C28H35F4NO2
SMILES: CCCCCCCCCCCCCCN(C(=O)c1cc(F)ccc1F)C(=O)c1cc(F)ccc1F
Mol. weight [g/mol]: 493.58

Physical Properties

Property code	Value	Unit	Source
gf	-555.12	kJ/mol	Joback Method
hf	-1136.14	kJ/mol	Joback Method
hfus	73.34	kJ/mol	Joback Method
hvap	97.39	kJ/mol	Joback Method
log10ws	-10.35		Crippen Method
logp	8.227		Crippen Method
mcvol	378.060	ml/mol	McGowan Method
pc	885.77	kPa	Joback Method
rinpol	3054.00		NIST Webbook
rinpol	3054.00		NIST Webbook
tb	1030.58	K	Joback Method
tc	1265.53	K	Joback Method
tf	642.93	K	Joback Method
vc	1.490	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1272.62	J/mol×K	1030.58	Joback Method
cpg	1288.79	J/mol×K	1069.74	Joback Method
cpg	1303.67	J/mol×K	1108.90	Joback Method
cpg	1317.36	J/mol×K	1148.06	Joback Method
cpg	1329.98	J/mol×K	1187.21	Joback Method
cpg	1341.65	J/mol×K	1226.37	Joback Method
cpg	1352.47	J/mol×K	1265.53	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407614&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
hvpap:	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
rinppl:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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