Benzamide, 2,5-difluoro-N-dodecyl-

Inchi: InChI=1S/C19H29F2NO/c1-2-3-4-5-6-7-8-9-10-11-14-22-19(23)17-15-16(20)12-13-18(17
InchiKey: XQIVFFNLXLITOP-UHFFFAOYSA-N
Formula: C19H29F2NO
SMILES: CCCCCCCCCCCCNC(=O)c1cc(F)ccc1F
Mol. weight [g/mol]: 325.44

Physical Properties

Property code	Value	Unit	Source
gf	-226.90	kJ/mol	Joback Method
hf	-673.23	kJ/mol	Joback Method
hfus	51.09	kJ/mol	Joback Method
hvap	73.04	kJ/mol	Joback Method
log10ws	-7.08		Crippen Method
logp	5.615		Crippen Method
mcvol	269.900	ml/mol	McGowan Method
pc	1317.52	kPa	Joback Method
rinpol	2379.00		NIST Webbook
rinpol	2379.00		NIST Webbook
tb	773.34	K	Joback Method
tc	959.32	K	Joback Method
tf	459.12	K	Joback Method
vc	1.069	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	814.08	J/mol×K	773.34	Joback Method
cpg	830.58	J/mol×K	804.34	Joback Method
cpg	846.17	J/mol×K	835.33	Joback Method
cpg	860.87	J/mol×K	866.33	Joback Method
cpg	874.72	J/mol×K	897.33	Joback Method
cpg	887.76	J/mol×K	928.32	Joback Method
cpg	900.02	J/mol×K	959.32	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407594&Units=SI

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