Benzamide, 2,6-difluoro-3-methyl-N-octyl-

Inchi: InChI=1S/C16H23F2NO/c1-3-4-5-6-7-8-11-19-16(20)14-13(17)10-9-12(2)15(14)18/h9-10
InchiKey: IJARWHIOAYSNMA-UHFFFAOYSA-N
Formula: C16H23F2NO
SMILES: CCCCCCCCNC(=O)c1c(F)ccc(C)c1F
Mol. weight [g/mol]: 283.36

Physical Properties

Property code	Value	Unit	Source
gf	-261.79	kJ/mol	Joback Method
hf	-622.78	kJ/mol	Joback Method
hfus	42.93	kJ/mol	Joback Method
hvap	67.02	kJ/mol	Joback Method
log10ws	-5.89		Crippen Method
logp	4.364		Crippen Method
mcvol	227.630	ml/mol	McGowan Method
pc	1623.29	kPa	Joback Method
rinpol	2158.00		NIST Webbook
rinpol	2158.00		NIST Webbook
tb	709.68	K	Joback Method
tc	896.49	K	Joback Method
tf	437.83	K	Joback Method
vc	0.900	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	643.99	J/mol×K	709.68	Joback Method
cpg	659.28	J/mol×K	740.82	Joback Method
cpg	673.74	J/mol×K	771.95	Joback Method
cpg	687.42	J/mol×K	803.09	Joback Method
cpg	700.32	J/mol×K	834.22	Joback Method
cpg	712.49	J/mol×K	865.36	Joback Method
cpg	723.94	J/mol×K	896.49	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=U407744&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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