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

Inchi: InChI=1S/C14H19F2NO/c1-3-4-5-6-9-17-14(18)12-11(15)8-7-10(2)13(12)16/h7-8H,3-6,9
InchiKey: ZFKUWNFMXYKDFA-UHFFFAOYSA-N
Formula: C14H19F2NO
SMILES: CCCCCCNC(=O)c1c(F)ccc(C)c1F
Mol. weight [g/mol]: 255.30

Physical Properties

Property code	Value	Unit	Source
gf	-278.63	kJ/mol	Joback Method
hf	-581.50	kJ/mol	Joback Method
hfus	37.75	kJ/mol	Joback Method
hvap	62.57	kJ/mol	Joback Method
log10ws	-5.05		Crippen Method
logp	3.583		Crippen Method
mcvol	199.450	ml/mol	McGowan Method
pc	1906.90	kPa	Joback Method
rinpol	1946.00		NIST Webbook
rinpol	1946.00		NIST Webbook
tb	663.92	K	Joback Method
tc	853.15	K	Joback Method
tf	415.29	K	Joback Method
vc	0.788	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	536.66	J/mol×K	663.92	Joback Method
cpg	551.03	J/mol×K	695.46	Joback Method
cpg	564.65	J/mol×K	727.00	Joback Method
cpg	577.52	J/mol×K	758.54	Joback Method
cpg	589.68	J/mol×K	790.08	Joback Method
cpg	601.15	J/mol×K	821.62	Joback Method
cpg	611.94	J/mol×K	853.15	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=U407741&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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