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

Inchi: InChI=1S/C15H21F2NO/c1-3-4-5-6-7-10-18-15(19)13-12(16)9-8-11(2)14(13)17/h8-9H,3-
InchiKey: NDVIGQCUVHFMSZ-UHFFFAOYSA-N
Formula: C15H21F2NO
SMILES: CCCCCCCNC(=O)c1c(F)ccc(C)c1F
Mol. weight [g/mol]: 269.33

Physical Properties

Property code	Value	Unit	Source
gf	-270.21	kJ/mol	Joback Method
hf	-602.14	kJ/mol	Joback Method
hfus	40.34	kJ/mol	Joback Method
hvap	64.79	kJ/mol	Joback Method
log10ws	-5.47		Crippen Method
logp	3.973		Crippen Method
mcvol	213.540	ml/mol	McGowan Method
pc	1756.54	kPa	Joback Method
rinpol	2056.00		NIST Webbook
rinpol	2056.00		NIST Webbook
tb	686.80	K	Joback Method
tc	874.61	K	Joback Method
tf	426.56	K	Joback Method
vc	0.845	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	589.69	J/mol×K	686.80	Joback Method
cpg	604.55	J/mol×K	718.10	Joback Method
cpg	618.61	J/mol×K	749.40	Joback Method
cpg	631.90	J/mol×K	780.70	Joback Method
cpg	644.46	J/mol×K	812.01	Joback Method
cpg	656.30	J/mol×K	843.31	Joback Method
cpg	667.44	J/mol×K	874.61	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407743&Units=SI
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

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