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

Inchi: InChI=1S/C15H21F2NO/c1-2-3-4-5-6-7-11-18-15(19)14-12(16)9-8-10-13(14)17/h8-10H,2
InchiKey: AHQXSEYIKCYOII-UHFFFAOYSA-N
Formula: C15H21F2NO
SMILES: CCCCCCCCNC(=O)c1c(F)cccc1F
Mol. weight [g/mol]: 269.33

Physical Properties

Property code	Value	Unit	Source
gf	-260.58	kJ/mol	Joback Method
hf	-590.67	kJ/mol	Joback Method
hfus	40.73	kJ/mol	Joback Method
hvap	64.13	kJ/mol	Joback Method
log10ws	-5.41		Crippen Method
logp	4.055		Crippen Method
mcvol	213.540	ml/mol	McGowan Method
pc	1778.84	kPa	Joback Method
rinpol	1886.00		NIST Webbook
rinpol	1886.00		NIST Webbook
tb	681.82	K	Joback Method
tc	868.78	K	Joback Method
tf	414.04	K	Joback Method
vc	0.845	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	590.24	J/mol×K	681.82	Joback Method
cpg	605.23	J/mol×K	712.98	Joback Method
cpg	619.40	J/mol×K	744.14	Joback Method
cpg	632.79	J/mol×K	775.30	Joback Method
cpg	645.42	J/mol×K	806.46	Joback Method
cpg	657.32	J/mol×K	837.62	Joback Method
cpg	668.52	J/mol×K	868.78	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=U415916&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