

3,4-Difluorobenzamide, N-(2-octyl)-

Inchi:	InChI=1S/C15H21F2NO/c1-3-4-5-6-7-11(2)18-15(19)12-8-9-13(16)14(17)10-12/h8-11H,3
InchiKey:	DHDAQNQJOQZWCB-UHFFFAOYSA-N
Formula:	C15H21F2NO
SMILES:	CCCCCCC(C)NC(=O)c1ccc(F)c(F)c1
Mol. weight [g/mol]:	269.33

Physical Properties

Property code	Value	Unit	Source
gf	-263.02	kJ/mol	Joback Method
hf	-595.95	kJ/mol	Joback Method
hfus	37.20	kJ/mol	Joback Method
hvap	63.74	kJ/mol	Joback Method
log10ws	-5.52		Crippen Method
logp	4.054		Crippen Method
mvol	213.540	ml/mol	McGowan Method
pc	1790.91	kPa	Joback Method
rinpol	1913.00		NIST Webbook
rinpol	1913.00		NIST Webbook
tb	681.38	K	Joback Method
tc	871.18	K	Joback Method
tf	399.04	K	Joback Method
vc	0.839	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	590.73	J/mol×K	681.38	Joback Method
cpg	605.97	J/mol×K	713.01	Joback Method
cpg	620.37	J/mol×K	744.65	Joback Method
cpg	633.95	J/mol×K	776.28	Joback Method
cpg	646.73	J/mol×K	807.91	Joback Method
cpg	658.77	J/mol×K	839.55	Joback Method
cpg	670.07	J/mol×K	871.18	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=U358123&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
rinpolar:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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