Benzamide, 3,4-difluoro-N-2-ethylhexyl-

Inchi: InChI=1S/C15H21F2NO/c1-3-5-6-11(4-2)10-18-15(19)12-7-8-13(16)14(17)9-12/h7-9,11H
InchiKey: KHFCULOIKKJIJE-UHFFFAOYSA-N
Formula: C15H21F2NO
SMILES: CCCCC(CC)CNC(=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	-5.17		Crippen Method
logp	3.911		Crippen Method
mcvol	213.540	ml/mol	McGowan Method
pc	1790.91	kPa	Joback Method
rinpol	1925.00		NIST Webbook
rinpol	1925.00		NIST Webbook
tb	681.38	K	Joback Method
tc	871.18	K	Joback Method
tf	399.04	K	Joback Method
vc	0.839	m3/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

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=U407795&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