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

Inchi: InChI=1S/C16H23F2NO/c1-4-6-7-12(5-2)10-19-16(20)14-13(17)9-8-11(3)15(14)18/h8-9,1

InchiKey: IIUKMRPCQRKXRA-UHFFFAOYSA-N

Formula: C16H23F2NO

SMILES: CCCCC(CC)CNC(=O)c1c(F)ccc(C)c1F

Mol. weight [g/mol]: 283.36

Physical Properties

Property code	Value	Unit	Source
gf	-264.23	kJ/mol	Joback Method
hf	-628.06	kJ/mol	Joback Method
hfus	39.40	kJ/mol	Joback Method
hvap	66.63	kJ/mol	Joback Method
log10ws	-5.64		Crippen Method
logp	4.219		Crippen Method
mcvol	227.630	ml/mol	McGowan Method
pc	1633.81	kPa	Joback Method
rinpol	2064.00		NIST Webbook
rinpol	2064.00		NIST Webbook
tb	709.24	K	Joback Method
tc	898.62	K	Joback Method
tf	422.83	K	Joback Method
vc	0.894	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	644.50	J/mol×K	709.24	Joback Method
cpg	660.02	J/mol×K	740.80	Joback Method
cpg	674.68	J/mol×K	772.37	Joback Method
cpg	688.53	J/mol×K	803.93	Joback Method
cpg	701.58	J/mol×K	835.50	Joback Method
cpg	713.85	J/mol×K	867.06	Joback Method
cpg	725.39	J/mol×K	898.62	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=U407742&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