3,4-Difluorobenzamide, N,N-di(2-ethylhexyl)-

Inchi: InChI=1S/C23H37F2NO/c1-5-9-11-18(7-3)16-26(17-19(8-4)12-10-6-2)23(27)20-13-14-21
InchiKey: JQBRFATXIBQCFR-UHFFFAOYSA-N
Formula: C23H37F2NO
SMILES: CCCCC(CC)CN(CC(CC)CCCC)C(=O)c1ccc(F)c(F)c1
Mol. weight [g/mol]: 381.54

Physical Properties

Property code	Value	Unit	Source
gf	-176.71	kJ/mol	Joback Method
hf	-752.29	kJ/mol	Joback Method
hfus	52.32	kJ/mol	Joback Method
hvap	76.77	kJ/mol	Joback Method
log10ws	-7.66		Crippen Method
logp	6.840		Crippen Method
mcvol	326.260	ml/mol	McGowan Method
pc	1015.53	kPa	Joback Method
rinpol	2324.00		NIST Webbook
rinpol	2324.00		NIST Webbook
tb	826.25	K	Joback Method
tc	1016.00	K	Joback Method
tf	454.01	K	Joback Method
vc	1.264	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1033.24	J/mol×K	826.25	Joback Method
cpg	1052.00	J/mol×K	857.87	Joback Method
cpg	1069.66	J/mol×K	889.50	Joback Method
cpg	1086.29	J/mol×K	921.12	Joback Method
cpg	1101.93	J/mol×K	952.75	Joback Method
cpg	1116.64	J/mol×K	984.37	Joback Method
cpg	1130.47	J/mol×K	1016.00	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358128&Units=SI

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