Benzamide, 2,3,4-trifluoro-N-(2-ethylhexyl)-

Inchi: InChI=1S/C15H20F3NO/c1-3-5-6-10(4-2)9-19-15(20)11-7-8-12(16)14(18)13(11)17/h7-8,1
InchiKey: PQPKSQYUTYLOMI-UHFFFAOYSA-N
Formula: C15H20F3NO
SMILES: CCCCC(CC)CNC(=O)c1ccc(F)c(F)c1F
Mol. weight [g/mol]: 287.32

Physical Properties

Property code	Value	Unit	Source
gf	-467.46	kJ/mol	Joback Method
hf	-803.53	kJ/mol	Joback Method
hfus	39.89	kJ/mol	Joback Method
hvap	63.59	kJ/mol	Joback Method
log10ws	-5.50		Crippen Method
logp	4.050		Crippen Method
mcvol	215.310	ml/mol	McGowan Method
pc	1703.31	kPa	Joback Method
rinpol	1836.00		NIST Webbook
rinpol	1836.00		NIST Webbook
tb	685.63	K	Joback Method
tc	869.82	K	Joback Method
tf	412.15	K	Joback Method
vc	0.857	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	598.10	J/mol×K	685.63	Joback Method
cpg	612.63	J/mol×K	716.33	Joback Method
cpg	626.39	J/mol×K	747.03	Joback Method
cpg	639.39	J/mol×K	777.72	Joback Method
cpg	651.66	J/mol×K	808.42	Joback Method
cpg	663.23	J/mol×K	839.12	Joback Method
cpg	674.11	J/mol×K	869.82	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=U407265&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