Benzamide, 2-trifluoromethyl-N-ethyl-N-hexyl-

Inchi: InChI=1S/C16H22F3NO/c1-3-5-6-9-12-20(4-2)15(21)13-10-7-8-11-14(13)16(17,18)19/h7
InchiKey: WOWYEBDBZYMSAQ-UHFFFAOYSA-N
Formula: C16H22F3NO
SMILES: CCCCCCN(CC)C(=O)c1ccccc1C(F)(F)F
Mol. weight [g/mol]: 301.35

Physical Properties

Property code	Value	Unit	Source
gf	-413.11	kJ/mol	Joback Method
hf	-790.64	kJ/mol	Joback Method
hfus	37.29	kJ/mol	Joback Method
hvap	59.19	kJ/mol	Joback Method
log10ws	-5.23		Crippen Method
logp	4.748		Crippen Method
mcvol	229.400	ml/mol	McGowan Method
pc	1609.00	kPa	Joback Method
rinpol	2007.00		NIST Webbook
rinpol	2007.00		NIST Webbook
tb	658.03	K	Joback Method
tc	840.69	K	Joback Method
tf	395.61	K	Joback Method
vc	0.890	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	637.22	J/mol×K	658.03	Joback Method
cpg	653.37	J/mol×K	688.47	Joback Method
cpg	668.57	J/mol×K	718.92	Joback Method
cpg	682.87	J/mol×K	749.36	Joback Method
cpg	696.33	J/mol×K	779.80	Joback Method
cpg	708.98	J/mol×K	810.24	Joback Method
cpg	720.88	J/mol×K	840.69	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=U415604&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