Benzamide, 3-trifluoromethyl-N-ethyl-N-octyl-

Inchi: InChI=1S/C18H26F3NO/c1-3-5-6-7-8-9-13-22(4-2)17(23)15-11-10-12-16(14-15)18(19,20
InchiKey: WHQITOURSNFZFK-UHFFFAOYSA-N
Formula: C18H26F3NO
SMILES: CCCCCCCCN(CC)C(=O)c1cccc(C(F)(F)F)c1
Mol. weight [g/mol]: 329.40

Physical Properties

Property code	Value	Unit	Source
gf	-396.27	kJ/mol	Joback Method
hf	-831.92	kJ/mol	Joback Method
hfus	42.47	kJ/mol	Joback Method
hvap	63.64	kJ/mol	Joback Method
log10ws	-6.07		Crippen Method
logp	5.528		Crippen Method
mcvol	257.580	ml/mol	McGowan Method
pc	1387.11	kPa	Joback Method
rinpol	2168.00		NIST Webbook
rinpol	2168.00		NIST Webbook
tb	703.79	K	Joback Method
tc	884.99	K	Joback Method
tf	418.15	K	Joback Method
vc	1.002	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	747.44	J/mol×K	703.79	Joback Method
cpg	764.20	J/mol×K	733.99	Joback Method
cpg	779.99	J/mol×K	764.19	Joback Method
cpg	794.87	J/mol×K	794.39	Joback Method
cpg	808.90	J/mol×K	824.59	Joback Method
cpg	822.12	J/mol×K	854.79	Joback Method
cpg	834.59	J/mol×K	884.99	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415577&Units=SI
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

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