Benzamide, 3-trifluoromethyl-N-ethyl-N-heptyl-

Inchi: InChI=1S/C17H24F3NO/c1-3-5-6-7-8-12-21(4-2)16(22)14-10-9-11-15(13-14)17(18,19)20
InchiKey: ASYDJKCUIZOFMW-UHFFFAOYSA-N
Formula: C17H24F3NO
SMILES: CCCCCCCN(CC)C(=O)c1cccc(C(F)(F)F)c1
Mol. weight [g/mol]: 315.37

Physical Properties

Property code	Value	Unit	Source
gf	-404.69	kJ/mol	Joback Method
hf	-811.28	kJ/mol	Joback Method
hfus	39.88	kJ/mol	Joback Method
hvap	61.42	kJ/mol	Joback Method
log10ws	-5.65		Crippen Method
logp	5.138		Crippen Method
mcvol	243.490	ml/mol	McGowan Method
pc	1491.89	kPa	Joback Method
rinpol	2083.00		NIST Webbook
rinpol	2083.00		NIST Webbook
tb	680.91	K	Joback Method
tc	862.62	K	Joback Method
tf	406.88	K	Joback Method
vc	0.947	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	691.76	J/mol×K	680.91	Joback Method
cpg	708.22	J/mol×K	711.20	Joback Method
cpg	723.73	J/mol×K	741.48	Joback Method
cpg	738.33	J/mol×K	771.77	Joback Method
cpg	752.08	J/mol×K	802.05	Joback Method
cpg	765.03	J/mol×K	832.34	Joback Method
cpg	777.23	J/mol×K	862.62	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415576&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