Benzamide, 3-trifluoromethyl-N-ethyl-N-hept-2-yl-

Inchi: InChI=1S/C17H24F3NO/c1-4-6-7-9-13(3)21(5-2)16(22)14-10-8-11-15(12-14)17(18,19)20

InchiKey: PQNHEJQLXMHPLA-UHFFFAOYSA-N

Formula: C17H24F3NO

SMILES: CCCCCC(C)N(CC)C(=O)c1cccc(C(F)(F)F)c1

Mol. weight [g/mol]: 315.37

Physical Properties

Property code	Value	Unit	Source
gf	-407.13	kJ/mol	Joback Method
hf	-816.56	kJ/mol	Joback Method
hfus	36.36	kJ/mol	Joback Method
hvap	61.03	kJ/mol	Joback Method
log10ws	-5.76		Crippen Method
logp	5.136		Crippen Method
mcvol	243.490	ml/mol	McGowan Method
pc	1501.15	kPa	Joback Method
rinpol	1961.00		NIST Webbook
rinpol	1961.00		NIST Webbook
tb	680.47	K	Joback Method
tc	864.77	K	Joback Method
tf	391.88	K	Joback Method
vc	0.941	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	692.22	J/mol×K	680.47	Joback Method
cpg	708.95	J/mol×K	711.19	Joback Method
cpg	724.68	J/mol×K	741.90	Joback Method
cpg	739.48	J/mol×K	772.62	Joback Method
cpg	753.40	J/mol×K	803.34	Joback Method
cpg	766.48	J/mol×K	834.06	Joback Method
cpg	778.79	J/mol×K	864.77	Joback Method

Sources

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=U415573&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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