Benzamide, 2,3,4-trifluoro-N-heptyl-

Inchi: InChI=1S/C14H18F3NO/c1-2-3-4-5-6-9-18-14(19)10-7-8-11(15)13(17)12(10)16/h7-8H,2-
InchiKey: TWYPRTVLADKWPB-UHFFFAOYSA-N
Formula: C14H18F3NO
SMILES: CCCCCCCNC(=O)c1ccc(F)c(F)c1F
Mol. weight [g/mol]: 273.29

Physical Properties

Property code	Value	Unit	Source
gf	-473.44	kJ/mol	Joback Method
hf	-777.61	kJ/mol	Joback Method
hfus	40.83	kJ/mol	Joback Method
hvap	61.75	kJ/mol	Joback Method
log10ws	-5.32		Crippen Method
logp	3.804		Crippen Method
mcvol	201.220	ml/mol	McGowan Method
pc	1834.11	kPa	Joback Method
rinpol	1826.00		NIST Webbook
rinpol	1826.00		NIST Webbook
tb	663.19	K	Joback Method
tc	845.70	K	Joback Method
tf	415.88	K	Joback Method
vc	0.806	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	544.64	J/mol×K	663.19	Joback Method
cpg	558.45	J/mol×K	693.61	Joback Method
cpg	571.54	J/mol×K	724.03	Joback Method
cpg	583.94	J/mol×K	754.45	Joback Method
cpg	595.66	J/mol×K	784.86	Joback Method
cpg	606.73	J/mol×K	815.28	Joback Method
cpg	617.16	J/mol×K	845.70	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407266&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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