Benzamide, pentafluoro-N-(hept-2-yl)-

Inchi: InChI=1S/C14H16F5NO/c1-3-4-5-6-7(2)20-14(21)8-9(15)11(17)13(19)12(18)10(8)16/h7H
InchiKey: DHRASMRLUZLFSE-UHFFFAOYSA-N
Formula: C14H16F5NO
SMILES: CCCCCC(C)NC(=O)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 309.27

Physical Properties

Property code	Value	Unit	Source
gf	-884.76	kJ/mol	Joback Method
hf	-1198.05	kJ/mol	Joback Method
hfus	42.69	kJ/mol	Joback Method
hvap	61.05	kJ/mol	Joback Method
log10ws	-6.10		Crippen Method
logp	4.081		Crippen Method
mcvol	204.760	ml/mol	McGowan Method
pc	1670.06	kPa	Joback Method
rinpol	1689.00		NIST Webbook
rinpol	1689.00		NIST Webbook
tb	671.25	K	Joback Method
tc	846.21	K	Joback Method
tf	427.10	K	Joback Method
vc	0.837	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	559.77	J/mol×K	671.25	Joback Method
cpg	572.54	J/mol×K	700.41	Joback Method
cpg	584.69	J/mol×K	729.57	Joback Method
cpg	596.22	J/mol×K	758.73	Joback Method
cpg	607.15	J/mol×K	787.89	Joback Method
cpg	617.49	J/mol×K	817.05	Joback Method
cpg	627.25	J/mol×K	846.21	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=U407940&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