

Pentafluoropropanamide, N-3-methylbutyl-

Inchi:	InChI=1S/C8H12F5NO/c1-5(2)3-4-14-6(15)7(9,10)8(11,12)13/h5H,3-4H2,1-2H3,(H,14,15)
InchiKey:	UHCIHGOYCUACPW-UHFFFAOYSA-N
Formula:	C8H12F5NO
SMILES:	CC(C)CCNC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	233.18

Physical Properties

Property code	Value	Unit	Source
gf	-993.86	kJ/mol	Joback Method
hf	-1270.89	kJ/mol	Joback Method
hfus	20.22	kJ/mol	Joback Method
hvap	39.52	kJ/mol	Joback Method
log10ws	-2.87		Crippen Method
logp	2.346		Crippen Method
mcvol	143.980	ml/mol	McGowan Method
pc	2291.52	kPa	Joback Method
rinpola	944.00		NIST Webbook
rinpola	944.00		NIST Webbook
tb	475.93	K	Joback Method
tc	636.89	K	Joback Method
tf	275.30	K	Joback Method
vc	0.587	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	349.29	J/mol×K	475.93	Joback Method
cpg	361.67	J/mol×K	502.76	Joback Method
cpg	373.36	J/mol×K	529.58	Joback Method
cpg	384.38	J/mol×K	556.41	Joback Method
cpg	394.76	J/mol×K	583.24	Joback Method
cpg	404.54	J/mol×K	610.07	Joback Method
cpg	413.74	J/mol×K	636.89	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407332&Units=SI

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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