

n-Heptafluoropropyl bromide

Other names:	Heptafluoropropyl bromide Heptafluoro-n-propyl bromide Propane, 1-bromo-1,1,2,2,3,3,3-heptafluoro- 1-bromo-1,1,2,2,3,3,3-heptafluoropropane
Inchi:	InChI=1S/C3BrF7/c4-2(7,8)1(5,6)3(9,10)11
InchiKey:	LANNRYWUUQMNPf-UHFFFAOYSA-N
Formula:	C3BrF7
SMILES:	FC(F)(F)C(F)(F)C(F)(F)Br
Mol. weight [g/mol]:	248.93
CAS:	422-85-5

Physical Properties

Property code	Value	Unit	Source
gf	-1366.45	kJ/mol	Joback Method
hf	-1477.94	kJ/mol	Joback Method
hfus	8.13	kJ/mol	Joback Method
hvap	19.10	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	3.172		Crippen Method
mcvol	83.020	ml/mol	McGowan Method
pc	3480.65	kPa	Joback Method
tb	285.00	K	NIST Webbook
tc	470.49	K	Joback Method
tf	194.76	K	Joback Method
vc	0.358	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	153.36	J/molxK	319.40	Joback Method
cpg	161.72	J/molxK	344.58	Joback Method
cpg	169.44	J/molxK	369.76	Joback Method
cpg	176.52	J/molxK	394.94	Joback Method
cpg	183.02	J/molxK	420.13	Joback Method

cpg	188.94	J/mol×K	445.31	Joback Method
cpg	194.33	J/mol×K	470.49	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C422855&Units=SI
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

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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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