

Propane, 1,2-dichloropentafluoro-2-(trifluoromethyl)-

Inchi:	InChI=1S/C4Cl2F8/c5-1(2(6,7)8,3(9,10)11)4(12,13)14
InchiKey:	SCNOJVKMNLBGCR-UHFFFAOYSA-N
Formula:	C4Cl2F8
SMILES:	FC(F)(F)C(Cl)(C(F)(F)F)C(F)(F)Cl
Mol. weight [g/mol]:	270.94
CAS:	354-91-6

Physical Properties

Property code	Value	Unit	Source
gf	-1588.18	kJ/mol	Joback Method
hf	-1761.25	kJ/mol	Joback Method
hfus	9.49	kJ/mol	Joback Method
hvap	21.55	kJ/mol	Joback Method
log10ws	-4.05		Crippen Method
logp	3.920		Crippen Method
mcvol	105.860	ml/mol	McGowan Method
pc	2603.08	kPa	Joback Method
tb	347.02	K	Joback Method
tc	497.76	K	Joback Method
tf	209.08	K	Joback Method
vc	0.458	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	210.51	J/mol×K	347.02	Joback Method
cpg	220.26	J/mol×K	372.14	Joback Method
cpg	229.22	J/mol×K	397.27	Joback Method
cpg	237.43	J/mol×K	422.39	Joback Method
cpg	244.93	J/mol×K	447.52	Joback Method
cpg	251.76	J/mol×K	472.64	Joback Method
cpg	257.95	J/mol×K	497.76	Joback Method

Sources

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=C354916&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
mccvol:	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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