1,1,1,4,5,5,5-heptafluoro-3-(pentafluoroethyl)-2,4-b

Other names: 2-Pentene, 1,1,1,4,5,5,5-heptafluoro-3-(pentafluoroethyl)-2,4-bis(trifluoromethyl)-
Inchi: InChI=1S/C9F18/c10-3(7(19,20)21,8(22,23)24)1(4(11,12)9(25,26)27)2(5(13,14)15)6(16,1
InchiKey: KJIGYKCIAQBHEL-UHFFFAOYSA-N
Formula: C9F18
SMILES: FC(F)(F)C(=C(C(F)(F)C(F)(F)F)C(F)(C(F)(F)F)C(F)(F)F)C(F)(F)F
Mol. weight [g/mol]: 450.07
CAS: 30320-26-4

Physical Properties

Property code	Value	Unit	Source
chl	-2982.30 ± 5.20	kJ/mol	NIST Webbook
gf	-3398.68	kJ/mol	Joback Method
hf	-3753.30 ± 5.30	kJ/mol	NIST Webbook
hfl	-3792.00 ± 5.30	kJ/mol	NIST Webbook
hfus	20.19	kJ/mol	Joback Method
hvap	38.70 ± 0.30	kJ/mol	NIST Webbook
log10ws	-7.04		Crippen Method
logp	6.438		Crippen Method
mcvol	165.230	ml/mol	McGowan Method
pc	1374.80	kPa	Joback Method
tb	373.49	K	Joback Method
tc	483.99	K	Joback Method
tf	185.75	K	Joback Method
vc	0.768	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	408.73	J/mol×K	373.49	Joback Method
cpg	422.19	J/mol×K	391.91	Joback Method
cpg	434.86	J/mol×K	410.32	Joback Method
cpg	446.77	J/mol×K	428.74	Joback Method
cpg	457.93	J/mol×K	447.16	Joback Method
cpg	468.39	J/mol×K	465.57	Joback Method

cpg	478.17	J/mol×K	483.99	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C30320264&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

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume