Methacrylic acid, 2,2,2-trichloroethyl ester

Inchi: InChI=1S/C6H7Cl3O2/c1-4(2)5(10)11-3-6(7,8)9/h1,3H2,2H3
InchiKey: IUGNCEABJSRDPG-UHFFFAOYSA-N
Formula: C6H7Cl3O2
SMILES: C=C(C)C(=O)OCC(Cl)(Cl)Cl
Mol. weight [g/mol]: 217.48

Physical Properties

Property code	Value	Unit	Source
gf	-187.94	kJ/mol	Joback Method
hf	-352.30	kJ/mol	Joback Method
hfus	16.67	kJ/mol	Joback Method
hvap	49.38	kJ/mol	Joback Method
log10ws	-2.61		Crippen Method
logp	2.476		Crippen Method
mcvol	135.260	ml/mol	McGowan Method
pc	3110.57	kPa	Joback Method
rinpol	1138.00		NIST Webbook
rinpol	1138.00		NIST Webbook
tb	518.59	K	Joback Method
tc	734.98	K	Joback Method
tf	306.00	K	Joback Method
vc	0.513	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.51	J/mol×K	518.59	Joback Method
cpg	266.35	J/mol×K	554.65	Joback Method
cpg	274.56	J/mol×K	590.72	Joback Method
cpg	282.17	J/mol×K	626.78	Joback Method
cpg	289.22	J/mol×K	662.85	Joback Method
cpg	295.75	J/mol×K	698.91	Joback Method
cpg	301.77	J/mol×K	734.98	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360690&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

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

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