Fumaric acid, isobutyl 2,2,2-trichloroethyl ester

Inchi: InChI=1S/C10H13Cl3O4/c1-7(2)5-16-8(14)3-4-9(15)17-6-10(11,12)13/h3-4,7H,5-6H2,1-2

InchiKey: VYCVEXWSKPJYKF-ONEGZZNKSA-N

Formula: C10H13Cl3O4

SMILES: CC(C)COC(=O)C=CC(=O)OCC(Cl)(Cl)Cl

Mol. weight [g/mol]: 303.57

Physical Properties

Property code	Value	Unit	Source
gf	-389.69	kJ/mol	Joback Method
hf	-683.36	kJ/mol	Joback Method
hfus	29.09	kJ/mol	Joback Method
hvap	67.59	kJ/mol	Joback Method
log10ws	-2.91		Crippen Method
logp	2.655		Crippen Method
mcvol	199.060	ml/mol	McGowan Method
pc	2229.20	kPa	Joback Method
rinpol	1718.00		NIST Webbook
rinpol	1718.00		NIST Webbook
tb	693.56	K	Joback Method
tc	906.02	K	Joback Method
tf	418.88	K	Joback Method
vc	0.753	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	474.88	J/mol×K	693.56	Joback Method
cpg	522.18	J/mol×K	870.61	Joback Method
cpg	514.12	J/mol×K	835.20	Joback Method
cpg	505.39	J/mol×K	799.79	Joback Method
cpg	495.96	J/mol×K	764.38	Joback Method
cpg	485.81	J/mol×K	728.97	Joback Method
cpg	529.61	J/mol×K	906.02	Joback Method
dvisc	0.0000960	Pa×s	693.56	Joback Method

dvisc	0.0001272	Pa×s	647.78	Joback Method
dvisc	0.0001758	Pa×s	602.00	Joback Method
dvisc	0.0002562	Pa×s	556.22	Joback Method
dvisc	0.0003997	Pa×s	510.44	Joback Method
dvisc	0.0006805	Pa×s	464.66	Joback Method
dvisc	0.0013016	Pa×s	418.88	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348502&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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