Fumaric acid, butyl 2,2,2-trichloroethyl ester

Inchi: InChI=1S/C10H13Cl3O4/c1-2-3-6-16-8(14)4-5-9(15)17-7-10(11,12)13/h4-5H,2-3,6-7H2,1
InchiKey: ZAVMYKKEQJIFPH-SNAWJCMRSA-N
Formula: C10H13Cl3O4
SMILES: CCCCOC(=O)C=CC(=O)OCC(Cl)(Cl)Cl
Mol. weight [g/mol]: 303.57

Physical Properties

Property code	Value	Unit	Source
gf	-387.25	kJ/mol	Joback Method
hf	-678.08	kJ/mol	Joback Method
hfus	32.61	kJ/mol	Joback Method
hvap	67.98	kJ/mol	Joback Method
log10ws	-3.15		Crippen Method
logp	2.799		Crippen Method
mcvol	199.060	ml/mol	McGowan Method
pc	2212.45	kPa	Joback Method
rinpol	1768.00		NIST Webbook
rinpol	1768.00		NIST Webbook
tb	694.00	K	Joback Method
tc	902.76	K	Joback Method
tf	433.88	K	Joback Method
vc	0.759	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	474.31	J/mol×K	694.00	Joback Method
cpg	520.88	J/mol×K	867.96	Joback Method
cpg	512.89	J/mol×K	833.17	Joback Method
cpg	504.28	J/mol×K	798.38	Joback Method
cpg	494.99	J/mol×K	763.59	Joback Method
cpg	485.01	J/mol×K	728.79	Joback Method
cpg	528.26	J/mol×K	902.76	Joback Method
dvisc	0.0001037	Pa×s	694.00	Joback Method

dvisc	0.0001346	Pa×s	650.65	Joback Method
dvisc	0.0001814	Pa×s	607.29	Joback Method
dvisc	0.0002560	Pa×s	563.94	Joback Method
dvisc	0.0003825	Pa×s	520.59	Joback Method
dvisc	0.0006148	Pa×s	477.23	Joback Method
dvisc	0.0010864	Pa×s	433.88	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348503&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