Fumaric acid, 2,4,4-trimethylpentyl 2,2-dichloroethyl ester

Inchi: InChI=1S/C14H22Cl2O4/c1-10(7-14(2,3)4)8-19-12(17)5-6-13(18)20-9-11(15)16/h5-6,10-

InchiKey: WJXWYWHMMBZEFD-AATRIKPKSA-N

Formula: C14H22Cl2O4

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

Mol. weight [g/mol]: 325.23

Physical Properties

Property code	Value	Unit	Source
gf	-346.52	kJ/mol	Joback Method
hf	-755.46	kJ/mol	Joback Method
hfus	31.73	kJ/mol	Joback Method
hvap	71.73	kJ/mol	Joback Method
log10ws	-3.69		Crippen Method
logp	3.505		Crippen Method
mcvol	243.180	ml/mol	McGowan Method
pc	1656.49	kPa	Joback Method
rinpol	1950.00		NIST Webbook
rinpol	1950.00		NIST Webbook
tb	747.21	K	Joback Method
tc	949.80	K	Joback Method
tf	419.04	K	Joback Method
vc	0.922	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	660.23	J/mol×K	747.21	Joback Method
cpg	674.28	J/mol×K	780.97	Joback Method
cpg	687.43	J/mol×K	814.74	Joback Method
cpg	699.71	J/mol×K	848.50	Joback Method
cpg	711.16	J/mol×K	882.27	Joback Method
cpg	721.82	J/mol×K	916.03	Joback Method
cpg	731.73	J/mol×K	949.80	Joback Method
dvisc	0.0013155	Pa×s	419.04	Joback Method

dvisc	0.0005756	Pa×s	473.74	Joback Method
dvisc	0.0002988	Pa×s	528.43	Joback Method
dvisc	0.0001754	Pa×s	583.12	Joback Method
dvisc	0.0001128	Pa×s	637.82	Joback Method
dvisc	0.0000778	Pa×s	692.52	Joback Method
dvisc	0.0000567	Pa×s	747.21	Joback Method

Sources

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=U405604&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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