Fumaric acid, 2,5-dichlorophenyl 2-methylpent-3-yl ester

Inchi: InChI=1S/C16H18Cl2O4/c1-4-13(10(2)3)21-15(19)7-8-16(20)22-14-9-11(17)5-6-12(14)18

InchiKey: UKMFENCIKXQMKM-BQYQJAHWSA-N

Formula: C16H18Cl2O4

SMILES: CCC(OC(=O)C=CC(=O)Oc1cc(Cl)ccc1Cl)C(C)C

Mol. weight [g/mol]: 345.22

Physical Properties

Property code	Value	Unit	Source
gf	-239.37	kJ/mol	Joback Method
hf	-574.40	kJ/mol	Joback Method
hfus	37.58	kJ/mol	Joback Method
hvap	81.07	kJ/mol	Joback Method
log10ws	-5.09		Crippen Method
logp	4.433		Crippen Method
mcvol	247.600	ml/mol	McGowan Method
pc	1784.86	kPa	Joback Method
rinpol	2244.00		NIST Webbook
rinpol	2244.00		NIST Webbook
tb	832.84	K	Joback Method
tc	1054.61	K	Joback Method
tf	490.62	K	Joback Method
vc	0.938	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	673.33	J/mol×K	832.84	Joback Method
cpg	726.26	J/mol×K	1017.65	Joback Method
cpg	717.62	J/mol×K	980.69	Joback Method
cpg	708.03	J/mol×K	943.73	Joback Method
cpg	697.48	J/mol×K	906.76	Joback Method
cpg	685.92	J/mol×K	869.80	Joback Method
cpg	733.98	J/mol×K	1054.61	Joback Method
dvisc	0.0000534	Pa×s	832.84	Joback Method

dvisc	0.0000689	Pa×s	775.80	Joback Method
dvisc	0.0000925	Pa×s	718.77	Joback Method
dvisc	0.0001306	Pa×s	661.73	Joback Method
dvisc	0.0001969	Pa×s	604.69	Joback Method
dvisc	0.0003233	Pa×s	547.66	Joback Method
dvisc	0.0005957	Pa×s	490.62	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405965&Units=SI

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