Fumaric acid, 2,4-dichlorophenyl 2-methylpent-3-yl ester

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

InchiKey: ZFVXWTUROXLRKB-BQYQJAHWSA-N

Formula: C16H18Cl2O4

SMILES: CCC(OC(=O)C=CC(=O)Oc1ccc(Cl)cc1Cl)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	2247.00		NIST Webbook
rinpol	2247.00		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=U405693&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