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

Inchi: InChI=1S/C15H16Cl2O4/c1-9(2)10(3)20-14(18)6-7-15(19)21-13-5-4-11(16)8-12(13)17/h4

InchiKey: OGYGXLXKIAPJHA-VOTSOKGWSA-N

Formula: C15H16Cl2O4

SMILES: CC(C)C(C)OC(=O)C=CC(=O)Oc1ccc(Cl)cc1Cl

Mol. weight [g/mol]: 331.19

Physical Properties

Property code	Value	Unit	Source
gf	-247.79	kJ/mol	Joback Method
hf	-553.76	kJ/mol	Joback Method
hfus	34.99	kJ/mol	Joback Method
hvap	78.85	kJ/mol	Joback Method
log10ws	-4.67		Crippen Method
logp	4.043		Crippen Method
mcvol	233.510	ml/mol	McGowan Method
pc	1938.95	kPa	Joback Method
rinpol	2166.00		NIST Webbook
rinpol	2166.00		NIST Webbook
tb	809.96	K	Joback Method
tc	1034.25	K	Joback Method
tf	479.35	K	Joback Method
vc	0.881	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	618.34	J/mol×K	809.96	Joback Method
cpg	630.62	J/mol×K	847.34	Joback Method
cpg	641.91	J/mol×K	884.72	Joback Method
cpg	652.21	J/mol×K	922.11	Joback Method
cpg	661.57	J/mol×K	959.49	Joback Method
cpg	670.00	J/mol×K	996.87	Joback Method
cpg	677.52	J/mol×K	1034.25	Joback Method
dvisc	0.0006577	Pa×s	479.35	Joback Method

dvisc	0.0003613	Pa×s	534.45	Joback Method
dvisc	0.0002220	Pa×s	589.55	Joback Method
dvisc	0.0001483	Pa×s	644.65	Joback Method
dvisc	0.0001055	Pa×s	699.76	Joback Method
dvisc	0.0000789	Pa×s	754.86	Joback Method
dvisc	0.0000614	Pa×s	809.96	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=U405692&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