Fumaric acid, 3-methylbutyl 2,3-dichlorophenyl ester

Inchi: InChI=1S/C15H16Cl2O4/c1-10(2)8-9-20-13(18)6-7-14(19)21-12-5-3-4-11(16)15(12)17/h3

InchiKey: DSAPGXLJRAVLHZ-VOTSOKGWSA-N

Formula: C15H16Cl2O4

SMILES: CC(C)CCOC(=O)C=CC(=O)Oc1cccc(Cl)c1Cl

Mol. weight [g/mol]: 331.19

Physical Properties

Property code	Value	Unit	Source
gf	-245.35	kJ/mol	Joback Method
hf	-548.48	kJ/mol	Joback Method
hfus	38.52	kJ/mol	Joback Method
hvap	79.24	kJ/mol	Joback Method
log10ws	-4.56		Crippen Method
logp	4.044		Crippen Method
mcvol	233.510	ml/mol	McGowan Method
pc	1925.36	kPa	Joback Method
rinpol	2266.00		NIST Webbook
rinpol	2266.00		NIST Webbook
tb	810.40	K	Joback Method
tc	1031.36	K	Joback Method
tf	494.35	K	Joback Method
vc	0.887	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	617.74	J/mol×K	810.40	Joback Method
cpg	668.95	J/mol×K	994.53	Joback Method
cpg	660.53	J/mol×K	957.71	Joback Method
cpg	651.22	J/mol×K	920.88	Joback Method
cpg	641.01	J/mol×K	884.05	Joback Method
cpg	629.86	J/mol×K	847.23	Joback Method
cpg	676.50	J/mol×K	1031.36	Joback Method
dvisc	0.0000669	Pa×s	810.40	Joback Method

dvisc	0.0000847	Pa×s	757.72	Joback Method
dvisc	0.0001110	Pa×s	705.05	Joback Method
dvisc	0.0001520	Pa×s	652.38	Joback Method
dvisc	0.0002200	Pa×s	599.70	Joback Method
dvisc	0.0003420	Pa×s	547.02	Joback Method
dvisc	0.0005841	Pa×s	494.35	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=U405553&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