Fumaric acid, 2,4,6-trichlorophenyl 3-methylbut-2-yl ester

Inchi: InChI=1S/C15H15Cl3O4/c1-8(2)9(3)21-13(19)4-5-14(20)22-15-11(17)6-10(16)7-12(15)18

InchiKey: HGZXTIPLXICXFC-SNAWJCMRSA-N

Formula: C15H15Cl3O4

SMILES: CC(C)C(C)OC(=O)C=CC(=O)Oc1c(Cl)cc(Cl)cc1Cl

Mol. weight [g/mol]: 365.64

Physical Properties

Property code	Value	Unit	Source
gf	-269.35	kJ/mol	Joback Method
hf	-580.97	kJ/mol	Joback Method
hfus	38.80	kJ/mol	Joback Method
hvap	83.89	kJ/mol	Joback Method
log10ws	-5.36		Crippen Method
logp	4.696		Crippen Method
mcvol	245.750	ml/mol	McGowan Method
pc	1853.11	kPa	Joback Method
rinpol	2256.00		NIST Webbook
rinpol	2256.00		NIST Webbook
tb	852.37	K	Joback Method
tc	1080.38	K	Joback Method
tf	521.79	K	Joback Method
vc	0.930	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	638.51	J/mol×K	852.37	Joback Method
cpg	683.97	J/mol×K	1042.38	Joback Method
cpg	676.78	J/mol×K	1004.38	Joback Method
cpg	668.66	J/mol×K	966.38	Joback Method
cpg	659.59	J/mol×K	928.37	Joback Method
cpg	649.54	J/mol×K	890.37	Joback Method
cpg	690.25	J/mol×K	1080.38	Joback Method
dvisc	0.0000538	Pa×s	852.37	Joback Method

dvisc	0.0000681	Pa×s	797.27	Joback Method
dvisc	0.0000893	Pa×s	742.18	Joback Method
dvisc	0.0001222	Pa×s	687.08	Joback Method
dvisc	0.0001767	Pa×s	631.98	Joback Method
dvisc	0.0002741	Pa×s	576.89	Joback Method
dvisc	0.0004665	Pa×s	521.79	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405949&Units=SI
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

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