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

Inchi: InChI=1S/C16H17Cl3O4/c1-4-13(9(2)3)22-14(20)5-6-15(21)23-16-11(18)7-10(17)8-12(16

InchiKey: ULNIYEKYZALERC-AATRIKPKSA-N

Formula: C16H17Cl3O4

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

Mol. weight [g/mol]: 379.66

Physical Properties

Property code	Value	Unit	Source
gf	-260.93	kJ/mol	Joback Method
hf	-601.61	kJ/mol	Joback Method
hfus	41.39	kJ/mol	Joback Method
hvap	86.12	kJ/mol	Joback Method
log10ws	-5.78		Crippen Method
logp	5.086		Crippen Method
mcvol	259.840	ml/mol	McGowan Method
pc	1708.95	kPa	Joback Method
rinpol	2336.00		NIST Webbook
rinpol	2336.00		NIST Webbook
tb	875.25	K	Joback Method
tc	1101.08	K	Joback Method
tf	533.06	K	Joback Method
vc	0.987	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	693.82	J/mol×K	875.25	Joback Method
cpg	740.47	J/mol×K	1063.44	Joback Method
cpg	733.09	J/mol×K	1025.80	Joback Method
cpg	724.76	J/mol×K	988.16	Joback Method
cpg	715.45	J/mol×K	950.53	Joback Method
cpg	705.15	J/mol×K	912.89	Joback Method
cpg	746.92	J/mol×K	1101.08	Joback Method
dvisc	0.0000467	Pa×s	875.25	Joback Method

dvisc	0.0000593	Pa×s	818.22	Joback Method
dvisc	0.0000780	Pa×s	761.19	Joback Method
dvisc	0.0001073	Pa×s	704.15	Joback Method
dvisc	0.0001562	Pa×s	647.12	Joback Method
dvisc	0.0002445	Pa×s	590.09	Joback Method
dvisc	0.0004211	Pa×s	533.06	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405950&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

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