Fumaric acid, 2,5-dichlorophenyl 3-methylbut-2-en-1-yl ester

Inchi: InChI=1S/C15H14Cl2O4/c1-10(2)7-8-20-14(18)5-6-15(19)21-13-9-11(16)3-4-12(13)17/h3

InchiKey: KKMVOORPVGODRV-AATRIKPKSA-N

Formula: C15H14Cl2O4

SMILES: CC(C)=CCOC(=O)C=CC(=O)Oc1cc(Cl)ccc1Cl

Mol. weight [g/mol]: 329.18

Physical Properties

Property code	Value	Unit	Source
gf	-171.24	kJ/mol	Joback Method
hf	-435.77	kJ/mol	Joback Method
hfus	40.93	kJ/mol	Joback Method
hvap	79.66	kJ/mol	Joback Method
log10ws	-4.66		Crippen Method
logp	3.964		Crippen Method
mcvol	229.210	ml/mol	McGowan Method
pc	2010.90	kPa	Joback Method
rinpol	2280.00		NIST Webbook
rinpol	2280.00		NIST Webbook
tb	814.88	K	Joback Method
tc	1042.21	K	Joback Method
tf	490.31	K	Joback Method
vc	0.875	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	590.33	J/mol×K	814.88	Joback Method
cpg	601.88	J/mol×K	852.77	Joback Method
cpg	612.54	J/mol×K	890.66	Joback Method
cpg	622.36	J/mol×K	928.55	Joback Method
cpg	631.38	J/mol×K	966.44	Joback Method
cpg	639.64	J/mol×K	1004.32	Joback Method
cpg	647.18	J/mol×K	1042.21	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405966&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
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