Fumaric acid, 2,4,6-trichlorophenyl 3-methylbut-2-en-1-yl ester

Inchi: InChI=1S/C15H13Cl3O4/c1-9(2)5-6-21-13(19)3-4-14(20)22-15-11(17)7-10(16)8-12(15)18

InchiKey: VTQFBEXHYFXHSG-ONEGZZNKSA-N

Formula: C15H13Cl3O4

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

Mol. weight [g/mol]: 363.62

Physical Properties

Property code	Value	Unit	Source
gf	-192.80	kJ/mol	Joback Method
hf	-462.98	kJ/mol	Joback Method
hfus	44.74	kJ/mol	Joback Method
hvap	84.71	kJ/mol	Joback Method
log10ws	-5.34		Crippen Method
logp	4.618		Crippen Method
mcvol	241.450	ml/mol	McGowan Method
pc	1920.30	kPa	Joback Method
rinpol	2374.00		NIST Webbook
rinpol	2374.00		NIST Webbook
tb	857.29	K	Joback Method
tc	1088.20	K	Joback Method
tf	532.75	K	Joback Method
vc	0.923	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	609.47	J/mol×K	857.29	Joback Method
cpg	619.89	J/mol×K	895.78	Joback Method
cpg	629.47	J/mol×K	934.26	Joback Method
cpg	638.23	J/mol×K	972.75	Joback Method
cpg	646.21	J/mol×K	1011.23	Joback Method
cpg	653.47	J/mol×K	1049.72	Joback Method
cpg	660.02	J/mol×K	1088.20	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=U405951&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
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