Glutaric acid, 3-methylbut-2-en-1-yl 2,4,5-trichlorophenyl ester

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

InchiKey: FPJKVLBMLXMJKM-UHFFFAOYSA-N

Formula: C16H17Cl3O4

SMILES: CC(C)=CCOC(=O)CCCC(=O)Oc1cc(Cl)c(Cl)cc1Cl

Mol. weight [g/mol]: 379.66

Physical Properties

Property code	Value	Unit	Source
gf	-264.60	kJ/mol	Joback Method
hf	-600.84	kJ/mol	Joback Method
hfus	47.13	kJ/mol	Joback Method
hvap	86.98	kJ/mol	Joback Method
log10ws	-5.91		Crippen Method
logp	5.232		Crippen Method
mcvol	259.840	ml/mol	McGowan Method
pc	1693.51	kPa	Joback Method
rinpol	2564.00		NIST Webbook
rinpol	2564.00		NIST Webbook
tb	876.01	K	Joback Method
tc	1098.62	K	Joback Method
tf	549.10	K	Joback Method
vc	1.000	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	692.32	J/mol×K	876.01	Joback Method
cpg	703.55	J/mol×K	913.11	Joback Method
cpg	713.82	J/mol×K	950.21	Joback Method
cpg	723.15	J/mol×K	987.31	Joback Method
cpg	731.57	J/mol×K	1024.42	Joback Method
cpg	739.10	J/mol×K	1061.52	Joback Method
cpg	745.76	J/mol×K	1098.62	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=U392159&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