Glutaric acid, 2,4,6-trichlorophenyl but-3-en-1-yl ester

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

InchiKey: MZEWEWXBTKDSOP-UHFFFAOYSA-N

Formula: C15H15Cl3O4

SMILES: C=CCCOC(=O)CCCC(=O)Oc1c(Cl)cc(Cl)cc1Cl

Mol. weight [g/mol]: 365.64

Physical Properties

Property code	Value	Unit	Source
gf	-256.85	kJ/mol	Joback Method
hf	-562.20	kJ/mol	Joback Method
hfus	44.36	kJ/mol	Joback Method
hvap	84.04	kJ/mol	Joback Method
log10ws	-5.49		Crippen Method
logp	4.842		Crippen Method
mcvol	245.750	ml/mol	McGowan Method
pc	1812.32	kPa	Joback Method
rinpol	2398.00		NIST Webbook
rinpol	2398.00		NIST Webbook
tb	845.77	K	Joback Method
tc	1064.43	K	Joback Method
tf	555.11	K	Joback Method
vc	0.944	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	637.78	J/mol×K	845.77	Joback Method
cpg	682.21	J/mol×K	1027.99	Joback Method
cpg	675.17	J/mol×K	991.54	Joback Method
cpg	667.22	J/mol×K	955.10	Joback Method
cpg	658.34	J/mol×K	918.66	Joback Method
cpg	648.53	J/mol×K	882.21	Joback Method
cpg	688.35	J/mol×K	1064.43	Joback Method
dvisc	0.0000787	Pa×s	845.77	Joback Method

dvisc	0.0000961	Pa×s	797.33	Joback Method
dvisc	0.0001205	Pa×s	748.88	Joback Method
dvisc	0.0001559	Pa×s	700.44	Joback Method
dvisc	0.0002096	Pa×s	652.00	Joback Method
dvisc	0.0002954	Pa×s	603.55	Joback Method
dvisc	0.0004420	Pa×s	555.11	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U394045&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

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