Glutaric acid, 1-cyclopentylethyl 2,4,6-trichlorophenyl ester

Inchi: InChI=1S/C18H21Cl3O4/c1-11(12-5-2-3-6-12)24-16(22)7-4-8-17(23)25-18-14(20)9-13(19

InchiKey: HTXYQXCXIUSLAQ-UHFFFAOYSA-N

Formula: C18H21Cl3O4

SMILES: CC(OC(=O)CCCC(=O)Oc1c(Cl)cc(Cl)cc1Cl)C1CCCC1

Mol. weight [g/mol]: 407.72

Physical Properties

Property code	Value	Unit	Source
gf	-285.32	kJ/mol	Joback Method
hf	-694.35	kJ/mol	Joback Method
hfus	43.83	kJ/mol	Joback Method
hvap	91.26	kJ/mol	Joback Method
log10ws	-6.65		Crippen Method
logp	5.844		Crippen Method
mcvol	281.460	ml/mol	McGowan Method
pc	1611.58	kPa	Joback Method
rinpol	2717.00		NIST Webbook
rinpol	2717.00		NIST Webbook
tb	932.57	K	Joback Method
tc	1165.25	K	Joback Method
tf	586.58	K	Joback Method
vc	1.065	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	823.58	J/mol×K	932.57	Joback Method
cpg	835.83	J/mol×K	971.35	Joback Method
cpg	846.72	J/mol×K	1010.13	Joback Method
cpg	856.29	J/mol×K	1048.91	Joback Method
cpg	864.58	J/mol×K	1087.69	Joback Method
cpg	871.61	J/mol×K	1126.47	Joback Method
cpg	877.41	J/mol×K	1165.25	Joback Method
dvisc	0.0004650	Pa×s	586.58	Joback Method

dvisc	0.0002904	Pa×s	644.25	Joback Method
dvisc	0.0001960	Pa×s	701.91	Joback Method
dvisc	0.0001404	Pa×s	759.58	Joback Method
dvisc	0.0001054	Pa×s	817.24	Joback Method
dvisc	0.0000822	Pa×s	874.90	Joback Method
dvisc	0.0000661	Pa×s	932.57	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405470&Units=SI

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