Glutaric acid, cyclopentyl 2,3-dichlorophenyl ester

Inchi: InChI=1S/C16H18Cl2O4/c17-12-7-3-8-13(16(12)18)22-15(20)10-4-9-14(19)21-11-5-1-2-6

InchiKey: CBNMCNDEPNFZAG-UHFFFAOYSA-N

Formula: C16H18Cl2O4

SMILES: O=C(CCCC(=O)OC1CCCC1)Oc1cccc(Cl)c1Cl

Mol. weight [g/mol]: 345.22

Physical Properties

Property code	Value	Unit	Source
gf	-278.16	kJ/mol	Joback Method
hf	-620.58	kJ/mol	Joback Method
hfus	38.36	kJ/mol	Joback Method
hvap	82.15	kJ/mol	Joback Method
log10ws	-5.37		Crippen Method
logp	4.555		Crippen Method
mcvol	241.040	ml/mol	McGowan Method
pc	1966.56	kPa	Joback Method
rinpol	2512.00		NIST Webbook
rinpol	2512.00		NIST Webbook
tb	844.84	K	Joback Method
tc	1074.85	K	Joback Method
tf	536.60	K	Joback Method
vc	0.910	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	688.23	J/mol×K	844.84	Joback Method
cpg	743.21	J/mol×K	1036.52	Joback Method
cpg	734.62	J/mol×K	998.18	Joback Method
cpg	724.85	J/mol×K	959.85	Joback Method
cpg	713.88	J/mol×K	921.51	Joback Method
cpg	701.69	J/mol×K	883.18	Joback Method
cpg	750.67	J/mol×K	1074.85	Joback Method
dvisc	0.0001089	Pa×s	844.84	Joback Method

dvisc	0.0001343	Pa×s	793.47	Joback Method
dvisc	0.0001706	Pa×s	742.09	Joback Method
dvisc	0.0002245	Pa×s	690.72	Joback Method
dvisc	0.0003086	Pa×s	639.35	Joback Method
dvisc	0.0004487	Pa×s	587.97	Joback Method
dvisc	0.0007008	Pa×s	536.60	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405399&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

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