Glutaric acid, 2,3-dichlorophenyl trans-4-tert-butylcyclohexyl ester

Inchi: InChI=1S/C21H28Cl2O4/c1-21(2,3)14-10-12-15(13-11-14)26-18(24)8-5-9-19(25)27-17-7

InchiKey: UXNIHVYSVFSRDN-UHFFFAOYSA-N

Formula: C21H28Cl2O4

SMILES: CC(C)(C)C1CCC(OC(=O)CCCC(=O)Oc2cccc(Cl)c2Cl)CC1

Mol. weight [g/mol]: 415.35

Physical Properties

Property code	Value	Unit	Source
gf	-253.03	kJ/mol	Joback Method
hf	-759.03	kJ/mol	Joback Method
hfus	42.87	kJ/mol	Joback Method
hvap	91.85	kJ/mol	Joback Method
log10ws	-6.98		Crippen Method
logp	6.217		Crippen Method
mcvol	311.490	ml/mol	McGowan Method
pc	1347.68	kPa	Joback Method
rinpol	3029.00		NIST Webbook
rinpol	3029.00		NIST Webbook
tb	955.61	K	Joback Method
tc	1188.95	K	Joback Method
tf	587.61	K	Joback Method
vc	1.171	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	986.84	J/mol×K	955.61	Joback Method
cpg	1042.53	J/mol×K	1150.06	Joback Method
cpg	1034.34	J/mol×K	1111.17	Joback Method
cpg	1024.73	J/mol×K	1072.28	Joback Method
cpg	1013.64	J/mol×K	1033.39	Joback Method
cpg	1001.04	J/mol×K	994.50	Joback Method
cpg	1049.37	J/mol×K	1188.95	Joback Method
dvisc	0.0000369	Pa×s	955.61	Joback Method

dvisc	0.0000472	Pa×s	894.28	Joback Method
dvisc	0.0000625	Pa×s	832.94	Joback Method
dvisc	0.0000866	Pa×s	771.61	Joback Method
dvisc	0.0001269	Pa×s	710.28	Joback Method
dvisc	0.0002000	Pa×s	648.94	Joback Method
dvisc	0.0003463	Pa×s	587.61	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=U393407&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