Glutaric acid, 2,3-dichlorophenyl 3-phenylpropyl ester

Inchi: InChI=1S/C20H20Cl2O4/c21-16-10-4-11-17(20(16)22)26-19(24)13-5-12-18(23)25-14-6-9

InchiKey: QHVADTMMFQZQKE-UHFFFAOYSA-N

Formula: C20H20Cl2O4

SMILES: O=C(CCCC(=O)Oc1cccc(Cl)c1Cl)OCCCc1ccccc1

Mol. weight [g/mol]: 395.28

Physical Properties

Property code	Value	Unit	Source
gf	-168.62	kJ/mol	Joback Method
hf	-527.09	kJ/mol	Joback Method
hfus	48.83	kJ/mol	Joback Method
hvap	93.07	kJ/mol	Joback Method
log10ws	-6.14		Crippen Method
logp	5.245		Crippen Method
mcvol	284.500	ml/mol	McGowan Method
pc	1615.47	kPa	Joback Method
rinpol	3043.00		NIST Webbook
rinpol	3043.00		NIST Webbook
tb	947.76	K	Joback Method
tc	1179.66	K	Joback Method
tf	597.20	K	Joback Method
vc	1.085	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	824.58	J/mol×K	947.76	Joback Method
cpg	869.01	J/mol×K	1141.01	Joback Method
cpg	862.49	J/mol×K	1102.36	Joback Method
cpg	854.83	J/mol×K	1063.71	Joback Method
cpg	845.98	J/mol×K	1025.06	Joback Method
cpg	835.91	J/mol×K	986.41	Joback Method
cpg	874.43	J/mol×K	1179.66	Joback Method
dvisc	0.0000424	Pa×s	947.76	Joback Method

dvisc	0.0000530	Pa×s	889.33	Joback Method
dvisc	0.0000685	Pa×s	830.91	Joback Method
dvisc	0.0000920	Pa×s	772.48	Joback Method
dvisc	0.0001296	Pa×s	714.05	Joback Method
dvisc	0.0001941	Pa×s	655.63	Joback Method
dvisc	0.0003147	Pa×s	597.20	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=U391781&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