

Glutaric acid, 2,3-dichlorophenyl diphenylmethyl ester

Inchi:	InChI=1S/C24H20Cl2O4/c25-19-13-7-14-20(23(19)26)29-21(27)15-8-16-22(28)30-24(17)
InchiKey:	QDZYYVMHOWDZKS-UHFFFAOYSA-N
Formula:	C24H20Cl2O4
SMILES:	O=C(CCCC(=O)OC(c1ccccc1)c1ccccc1)Oc1cccc(Cl)c1Cl
Mol. weight [g/mol]:	443.32

Physical Properties

Property code	Value	Unit	Source
gf	-24.97	kJ/mol	Joback Method
hf	-378.40	kJ/mol	Joback Method
hfus	49.71	kJ/mol	Joback Method
hvap	103.86	kJ/mol	Joback Method
log10ws	-7.48		Crippen Method
logp	6.402		Crippen Method
mvol	317.100	ml/mol	McGowan Method
pc	1558.58	kPa	Joback Method
rinpol	3356.00		NIST Webbook
rinpol	3356.00		NIST Webbook
tb	1065.52	K	Joback Method
tc	1320.89	K	Joback Method
tf	653.70	K	Joback Method
vc	1.196	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	944.83	J/molxK	1065.52	Joback Method
cpg	953.84	J/molxK	1108.08	Joback Method
cpg	961.44	J/molxK	1150.64	Joback Method
cpg	967.71	J/molxK	1193.21	Joback Method
cpg	972.74	J/molxK	1235.77	Joback Method
cpg	976.62	J/molxK	1278.33	Joback Method
cpg	979.43	J/molxK	1320.89	Joback Method
dvisc	0.0001942	Paxs	653.70	Joback Method

dvisc	0.0001137	Paxs	722.34	Joback Method
dvisc	0.0000730	Paxs	790.97	Joback Method
dvisc	0.0000503	Paxs	859.61	Joback Method
dvisc	0.0000367	Paxs	928.25	Joback Method
dvisc	0.0000279	Paxs	996.88	Joback Method
dvisc	0.0000220	Paxs	1065.52	Joback Method

Sources

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=U393350&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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