

Glutaric acid, 2,4,6-trichlorophenyl 4-methylpent-2-yl ester

Inchi:	InChI=1S/C17H21Cl3O4/c1-10(2)7-11(3)23-15(21)5-4-6-16(22)24-17-13(19)8-12(18)9-14
InchiKey:	QIHSGBMOLNPRRW-UHFFFAOYSA-N
Formula:	C17H21Cl3O4
SMILES:	CC(C)CC(C)OC(=O)CCCC(=O)Oc1c(Cl)cc(Cl)cc1Cl
Mol. weight [g/mol]:	395.70

Physical Properties

Property code	Value	Unit	Source
gf	-332.73	kJ/mol	Joback Method
hf	-739.47	kJ/mol	Joback Method
hfus	43.78	kJ/mol	Joback Method
hvap	88.39	kJ/mol	Joback Method
log10ws	-6.34		Crippen Method
logp	5.700		Crippen Method
mcvol	278.230	ml/mol	McGowan Method
pc	1517.57	kPa	Joback Method
rinpol	2439.00		NIST Webbook
rinpol	2439.00		NIST Webbook
tb	893.97	K	Joback Method
tc	1113.16	K	Joback Method
tf	549.41	K	Joback Method
vc	1.062	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	778.04	J/molxK	893.97	Joback Method
cpg	790.01	J/molxK	930.50	Joback Method
cpg	800.84	J/molxK	967.03	Joback Method
cpg	810.55	J/molxK	1003.56	Joback Method
cpg	819.14	J/molxK	1040.10	Joback Method
cpg	826.63	J/molxK	1076.63	Joback Method
cpg	833.02	J/molxK	1113.16	Joback Method
dvisc	0.0004110	Paxs	549.41	Joback Method

dvisc	0.0002402	Paxs	606.84	Joback Method
dvisc	0.0001541	Paxs	664.26	Joback Method
dvisc	0.0001061	Paxs	721.69	Joback Method
dvisc	0.0000772	Paxs	779.12	Joback Method
dvisc	0.0000586	Paxs	836.54	Joback Method
dvisc	0.0000461	Paxs	893.97	Joback Method

Sources

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=U392501&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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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