

Glutaric acid, 2,3-dichlorophenyl but-3-en-1-yl ester

Inchi:	InChI=1S/C15H16Cl2O4/c1-2-3-10-20-13(18)8-5-9-14(19)21-12-7-4-6-11(16)15(12)17/h2
InchiKey:	QNZRGZSZJXAUSS-UHFFFAOYSA-N
Formula:	C15H16Cl2O4
SMILES:	C=CCCOC(=O)CCCC(=O)Oc1cccc(Cl)c1Cl
Mol. weight [g/mol]:	331.19

Physical Properties

Property code	Value	Unit	Source
gf	-235.29	kJ/mol	Joback Method
hf	-534.99	kJ/mol	Joback Method
hfus	40.56	kJ/mol	Joback Method
hvap	79.00	kJ/mol	Joback Method
log10ws	-4.80		Crippen Method
logp	4.188		Crippen Method
mvol	233.510	ml/mol	McGowan Method
pc	1895.30	kPa	Joback Method
rinpol	2345.00		NIST Webbook
rinpol	2345.00		NIST Webbook
tb	803.36	K	Joback Method
tc	1017.75	K	Joback Method
tf	512.67	K	Joback Method
vc	0.894	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	617.36	J/molxK	803.36	Joback Method
cpg	629.29	J/molxK	839.09	Joback Method
cpg	640.29	J/molxK	874.82	Joback Method
cpg	650.37	J/molxK	910.55	Joback Method
cpg	659.54	J/molxK	946.29	Joback Method
cpg	667.82	J/molxK	982.02	Joback Method
cpg	675.22	J/molxK	1017.75	Joback Method
dvisc	0.0005863	Paxs	512.67	Joback Method

dvisc	0.0003741	Paxs	561.12	Joback Method
dvisc	0.0002564	Paxs	609.57	Joback Method
dvisc	0.0001858	Paxs	658.01	Joback Method
dvisc	0.0001407	Paxs	706.46	Joback Method
dvisc	0.0001104	Paxs	754.91	Joback Method
dvisc	0.0000892	Paxs	803.36	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U394043&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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