

Glutaric acid, 3-methylbut-2-yl 2,3-dichlorophenyl ester

Inchi:	InChI=1S/C16H20Cl2O4/c1-10(2)11(3)21-14(19)8-5-9-15(20)22-13-7-4-6-12(17)16(13)18
InchiKey:	OHUXOObTTDIUJW-UHFFFAOYSA-N
Formula:	C16H20Cl2O4
SMILES:	CC(C)C(C)OC(=O)CCCC(=O)Oc1cccc(Cl)c1Cl
Mol. weight [g/mol]:	347.23

Physical Properties

Property code	Value	Unit	Source
gf	-319.59	kJ/mol	Joback Method
hf	-691.62	kJ/mol	Joback Method
hfus	37.38	kJ/mol	Joback Method
hvap	81.12	kJ/mol	Joback Method
log10ws	-5.24		Crippen Method
logp	4.657		Crippen Method
mvol	251.900	ml/mol	McGowan Method
pc	1708.95	kPa	Joback Method
rinpol	2318.00		NIST Webbook
rinpol	2318.00		NIST Webbook
tb	828.68	K	Joback Method
tc	1044.31	K	Joback Method
tf	495.70	K	Joback Method
vc	0.958	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	700.03	J/molxK	828.68	Joback Method
cpg	713.11	J/molxK	864.62	Joback Method
cpg	725.12	J/molxK	900.56	Joback Method
cpg	736.06	J/molxK	936.49	Joback Method
cpg	745.95	J/molxK	972.43	Joback Method
cpg	754.80	J/molxK	1008.37	Joback Method
cpg	762.63	J/molxK	1044.31	Joback Method
dvisc	0.0006451	Paxs	495.70	Joback Method

dvisc	0.0003577	Paxs	551.20	Joback Method
dvisc	0.0002210	Paxs	606.69	Joback Method
dvisc	0.0001480	Paxs	662.19	Joback Method
dvisc	0.0001054	Paxs	717.69	Joback Method
dvisc	0.0000789	Paxs	773.18	Joback Method
dvisc	0.0000613	Paxs	828.68	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391985&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cp_g:	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
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
m_{cvol}:	McGowan's characteristic volume
pc:	Critical Pressure
rin_{pol}:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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