

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

Inchi:	InChI=1S/C12H20Cl2O4/c1-8(2)9(3)18-12(16)6-4-5-11(15)17-7-10(13)14/h8-10H,4-7H2,
InchiKey:	PELKZLOXQRMYOE-UHFFFAOYSA-N
Formula:	C12H20Cl2O4
SMILES:	CC(C)C(C)OC(=O)CCCC(=O)OCC(Cl)Cl
Mol. weight [g/mol]:	299.19

Physical Properties

Property code	Value	Unit	Source
gf	-448.86	kJ/mol	Joback Method
hf	-827.93	kJ/mol	Joback Method
hfus	30.24	kJ/mol	Joback Method
hvap	68.22	kJ/mol	Joback Method
log10ws	-3.35		Crippen Method
logp	3.091		Crippen Method
mvol	219.300	ml/mol	McGowan Method
pc	1845.16	kPa	Joback Method
rinpol	1766.00		NIST Webbook
rinpol	1766.00		NIST Webbook
tb	700.08	K	Joback Method
tc	894.49	K	Joback Method
tf	384.16	K	Joback Method
vc	0.836	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	574.60	J/molxK	700.08	Joback Method
cpg	588.30	J/molxK	732.48	Joback Method
cpg	601.20	J/molxK	764.88	Joback Method
cpg	613.32	J/molxK	797.29	Joback Method
cpg	624.66	J/molxK	829.69	Joback Method
cpg	635.22	J/molxK	862.09	Joback Method
cpg	645.02	J/molxK	894.49	Joback Method
dvisc	0.0021572	Paxs	384.16	Joback Method

dvisc	0.0009443	Paxs	436.81	Joback Method
dvisc	0.0004937	Paxs	489.47	Joback Method
dvisc	0.0002928	Paxs	542.12	Joback Method
dvisc	0.0001905	Paxs	594.77	Joback Method
dvisc	0.0001329	Paxs	647.43	Joback Method
dvisc	0.0000979	Paxs	700.08	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393537&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
hvap:	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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