

Glutaric acid, 2,2-dichloroethyl 4-chlorobenzyl ester

Inchi:	InChI=1S/C14H15Cl3O4/c15-11-6-4-10(5-7-11)8-20-13(18)2-1-3-14(19)21-9-12(16)17/h
InchiKey:	ADVCWFNLFATVFI-UHFFFAOYSA-N
Formula:	C14H15Cl3O4
SMILES:	O=C(CCCC(=O)OCC(Cl)Cl)OCc1ccc(Cl)cc1
Mol. weight [g/mol]:	353.62

Physical Properties

Property code	Value	Unit	Source
gf	-336.29	kJ/mol	Joback Method
hf	-649.33	kJ/mol	Joback Method
hfus	40.31	kJ/mol	Joback Method
hvap	80.77	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	3.900		Crippen Method
mvol	235.960	ml/mol	McGowan Method
pc	1963.07	kPa	Joback Method
rinpol	2445.00		NIST Webbook
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tb	815.81	K	Joback Method
tc	1035.01	K	Joback Method
tf	505.56	K	Joback Method
vc	0.900	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	613.50	J/molxK	815.81	Joback Method
cpg	624.75	J/molxK	852.34	Joback Method
cpg	635.03	J/molxK	888.88	Joback Method
cpg	644.34	J/molxK	925.41	Joback Method
cpg	652.70	J/molxK	961.95	Joback Method
cpg	660.14	J/molxK	998.48	Joback Method
cpg	666.65	J/molxK	1035.01	Joback Method
dvisc	0.0006721	Paxs	505.56	Joback Method

dvisc	0.0003947	Paxs	557.27	Joback Method
dvisc	0.0002538	Paxs	608.98	Joback Method
dvisc	0.0001748	Paxs	660.68	Joback Method
dvisc	0.0001272	Paxs	712.39	Joback Method
dvisc	0.0000965	Paxs	764.10	Joback Method
dvisc	0.0000759	Paxs	815.81	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391726&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

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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