

Glutaric acid, 2,2-dichloroethyl diphenylmethyl ester

Inchi:	InChI=1S/C20H20Cl2O4/c21-17(22)14-25-18(23)12-7-13-19(24)26-20(15-8-3-1-4-9-15)1
InchiKey:	PFXPMXQLJJAOLO-UHFFFAOYSA-N
Formula:	C20H20Cl2O4
SMILES:	O=C(CCCC(=O)OC(c1ccccc1)c1ccccc1)OCC(Cl)Cl
Mol. weight [g/mol]:	395.28

Physical Properties

Property code	Value	Unit	Source
gf	-154.24	kJ/mol	Joback Method
hf	-514.71	kJ/mol	Joback Method
hfus	42.56	kJ/mol	Joback Method
hvap	90.97	kJ/mol	Joback Method
log10ws	-5.60		Crippen Method
logp	4.836		Crippen Method
mvol	284.500	ml/mol	McGowan Method
pc	1676.91	kPa	Joback Method
rinpol	2783.00		NIST Webbook
rinpol	2783.00		NIST Webbook
tb	936.92	K	Joback Method
tc	1172.40	K	Joback Method
tf	542.16	K	Joback Method
vc	1.073	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	828.57	J/molxK	936.92	Joback Method
cpg	874.65	J/molxK	1133.16	Joback Method
cpg	867.81	J/molxK	1093.91	Joback Method
cpg	859.84	J/molxK	1054.66	Joback Method
cpg	850.69	J/molxK	1015.41	Joback Method
cpg	840.28	J/molxK	976.17	Joback Method
cpg	880.43	J/molxK	1172.40	Joback Method
dvisc	0.0000338	Paxs	936.92	Joback Method

dvisc	0.0000445	Paxs	871.13	Joback Method
dvisc	0.0000613	Paxs	805.33	Joback Method
dvisc	0.0000894	Paxs	739.54	Joback Method
dvisc	0.0001404	Paxs	673.75	Joback Method
dvisc	0.0002429	Paxs	607.95	Joback Method
dvisc	0.0004804	Paxs	542.16	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393342&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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