

Glutaric acid, di(2-(2,4-dichlorophenyl)ethyl) ester

Inchi:	InChI=1S/C21H20Cl4O4/c22-16-6-4-14(18(24)12-16)8-10-28-20(26)2-1-3-21(27)29-11-9
InchiKey:	IPNVQUAMAKOXMP-UHFFFAOYSA-N
Formula:	C21H20Cl4O4
SMILES:	O=C(CCCC(=O)OCCc1ccc(Cl)cc1Cl)OCCc1ccc(Cl)cc1Cl
Mol. weight [g/mol]:	478.19

Physical Properties

Property code	Value	Unit	Source
gf	-203.32	kJ/mol	Joback Method
hf	-602.15	kJ/mol	Joback Method
hfus	59.03	kJ/mol	Joback Method
hvap	105.39	kJ/mol	Joback Method
log10ws	-7.28		Crippen Method
logp	6.342		Crippen Method
mcvol	323.070	ml/mol	McGowan Method
pc	1384.02	kPa	Joback Method
rinpol	3516.00		NIST Webbook
rinpol	3516.00		NIST Webbook
tb	1055.46	K	Joback Method
tc	1298.61	K	Joback Method
tf	693.35	K	Joback Method
vc	1.240	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	915.45	J/molxK	1055.46	Joback Method
cpg	923.88	J/molxK	1095.99	Joback Method
cpg	930.97	J/molxK	1136.51	Joback Method
cpg	936.74	J/molxK	1177.04	Joback Method
cpg	941.23	J/molxK	1217.56	Joback Method
cpg	944.50	J/molxK	1258.09	Joback Method
cpg	946.57	J/molxK	1298.61	Joback Method
dvisc	0.0001597	Paxs	693.35	Joback Method

dvisc	0.0001057	Paxs	753.70	Joback Method
dvisc	0.0000744	Paxs	814.05	Joback Method
dvisc	0.0000550	Paxs	874.40	Joback Method
dvisc	0.0000422	Paxs	934.76	Joback Method
dvisc	0.0000335	Paxs	995.11	Joback Method
dvisc	0.0000273	Paxs	1055.46	Joback Method

Sources

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=U377395&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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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