

Glutaric acid, cyclohexylmethyl 2,4-dichlorophenyl ester

Inchi: InChI=1S/C18H22Cl2O4/c19-14-9-10-16(15(20)11-14)24-18(22)8-4-7-17(21)23-12-13-5-
InchiKey: MJKWYLSHHFNSDA-UHFFFAOYSA-N
Formula: C18H22Cl2O4
SMILES: O=C(CCCC(=O)Oc1ccc(Cl)cc1Cl)OCC1CCCCC1
Mol. weight [g/mol]: 373.27

Physical Properties

Property code	Value	Unit	Source
gf	-273.42	kJ/mol	Joback Method
hf	-668.02	kJ/mol	Joback Method
hfus	41.44	kJ/mol	Joback Method
hvap	86.77	kJ/mol	Joback Method
log10ws	-5.86		Crippen Method
logp	5.193		Crippen Method
mvol	269.220	ml/mol	McGowan Method
pc	1704.71	kPa	Joback Method
rinpol	2733.00		NIST Webbook
rinpol	2733.00		NIST Webbook
tb	894.87	K	Joback Method
tc	1125.18	K	Joback Method
tf	555.62	K	Joback Method
vc	1.014	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	805.69	J/molxK	894.87	Joback Method
cpg	860.34	J/molxK	1086.79	Joback Method
cpg	852.22	J/molxK	1048.41	Joback Method
cpg	842.72	J/molxK	1010.02	Joback Method
cpg	831.82	J/molxK	971.64	Joback Method
cpg	819.49	J/molxK	933.25	Joback Method
cpg	867.11	J/molxK	1125.18	Joback Method
dvisc	0.0000568	Paxs	894.87	Joback Method

dvisc	0.0000720	Paxs	838.33	Joback Method
dvisc	0.0000943	Paxs	781.79	Joback Method
dvisc	0.0001290	Paxs	725.24	Joback Method
dvisc	0.0001861	Paxs	668.70	Joback Method
dvisc	0.0002871	Paxs	612.16	Joback Method
dvisc	0.0004838	Paxs	555.62	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391855&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

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
m_{cvol}:	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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