

Glutaric acid, di(2-chloro-5-methylphenyl) ester

Inchi: InChI=1S/C19H18Cl2O4/c1-12-6-8-14(20)16(10-12)24-18(22)4-3-5-19(23)25-17-11-13(2)
InchiKey: MKTYSQOZKQLKGN-UHFFFAOYSA-N
Formula: C19H18Cl2O4
SMILES: Cc1ccc(Cl)c(OC(=O)CCCC(=O)Oc2cc(C)ccc2Cl)c1
Mol. weight [g/mol]: 381.25

Physical Properties

Property code	Value	Unit	Source
gf	-196.30	kJ/mol	Joback Method
hf	-529.39	kJ/mol	Joback Method
hfus	45.46	kJ/mol	Joback Method
hvap	92.17	kJ/mol	Joback Method
log10ws	-6.49		Crippen Method
logp	5.292		Crippen Method
mcvol	270.410	ml/mol	McGowan Method
pc	1704.71	kPa	Joback Method
rinpol	2917.00		NIST Webbook
rinpol	2917.00		NIST Webbook
tb	934.84	K	Joback Method
tc	1169.45	K	Joback Method
tf	610.97	K	Joback Method
vc	1.030	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	764.29	J/mol×K	934.84	Joback Method
cpg	775.30	J/mol×K	973.94	Joback Method
cpg	785.03	J/mol×K	1013.04	Joback Method
cpg	793.48	J/mol×K	1052.15	Joback Method
cpg	800.70	J/mol×K	1091.25	Joback Method
cpg	806.69	J/mol×K	1130.35	Joback Method
cpg	811.48	J/mol×K	1169.45	Joback Method
dvisc	0.0002867	Pa×s	610.97	Joback Method

dvisc	0.0001914	Pa×s	664.95	Joback Method
dvisc	0.0001358	Pa×s	718.93	Joback Method
dvisc	0.0001011	Pa×s	772.90	Joback Method
dvisc	0.0000782	Pa×s	826.88	Joback Method
dvisc	0.0000624	Pa×s	880.86	Joback Method
dvisc	0.0000511	Pa×s	934.84	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=U359342&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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