

Glutaric acid, di(4-chloro-2-methoxyphenyl) ester

Inchi:	InChI=1S/C19H18Cl2O6/c1-24-16-10-12(20)6-8-14(16)26-18(22)4-3-5-19(23)27-15-9-7-
InchiKey:	ZNELHFVDPOZCRQ-UHFFFAOYSA-N
Formula:	C19H18Cl2O6
SMILES:	COc1cc(Cl)ccc1OC(=O)CCCC(=O)Oc1ccc(Cl)cc1OC
Mol. weight [g/mol]:	413.25

Physical Properties

Property code	Value	Unit	Source
gf	-406.30	kJ/mol	Joback Method
hf	-793.83	kJ/mol	Joback Method
hfus	47.84	kJ/mol	Joback Method
hvap	96.99	kJ/mol	Joback Method
log10ws	-5.78		Crippen Method
logp	4.692		Crippen Method
mvol	282.150	ml/mol	McGowan Method
pc	1657.84	kPa	Joback Method
rinpol	3119.00		NIST Webbook
rinpol	3119.00		NIST Webbook
tb	979.68	K	Joback Method
tc	1213.79	K	Joback Method
tf	655.43	K	Joback Method
vc	1.065	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	813.99	J/molxK	979.68	Joback Method
cpg	823.08	J/molxK	1018.70	Joback Method
cpg	830.56	J/molxK	1057.72	Joback Method
cpg	836.43	J/molxK	1096.74	Joback Method
cpg	840.66	J/molxK	1135.75	Joback Method
cpg	843.23	J/molxK	1174.77	Joback Method
cpg	844.13	J/molxK	1213.79	Joback Method
dvisc	0.0001487	Paxs	655.43	Joback Method

dvisc	0.0001015	Paxs	709.47	Joback Method
dvisc	0.0000732	Paxs	763.51	Joback Method
dvisc	0.0000550	Paxs	817.56	Joback Method
dvisc	0.0000429	Paxs	871.60	Joback Method
dvisc	0.0000344	Paxs	925.64	Joback Method
dvisc	0.0000283	Paxs	979.68	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393917&Units=SI

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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