

Glutaric acid, 3-chlorophenyl 2-isopropoxyphenyl ester

Inchi:	InChI=1S/C20H21ClO5/c1-14(2)24-17-9-3-4-10-18(17)26-20(23)12-6-11-19(22)25-16-8-5
InchiKey:	MTSKXBUFGZCBJG-UHFFFAOYSA-N
Formula:	C20H21ClO5
SMILES:	CC(C)Oc1ccccc1OC(=O)CCCC(=O)Oc1cccc(Cl)c1
Mol. weight [g/mol]:	376.83

Physical Properties

Property code	Value	Unit	Source
gf	-264.13	kJ/mol	Joback Method
hf	-648.85	kJ/mol	Joback Method
hfus	42.30	kJ/mol	Joback Method
hvap	90.71	kJ/mol	Joback Method
log10ws	-5.92		Crippen Method
logp	4.808		Crippen Method
mcvol	278.130	ml/mol	McGowan Method
pc	1652.46	kPa	Joback Method
rinpol	2747.00		NIST Webbook
rinpol	2747.00		NIST Webbook
tb	932.31	K	Joback Method
tc	1162.42	K	Joback Method
tf	574.51	K	Joback Method
vc	1.048	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	830.21	J/molxK	932.31	Joback Method
cpg	842.18	J/molxK	970.66	Joback Method
cpg	852.71	J/molxK	1009.01	Joback Method
cpg	861.82	J/molxK	1047.36	Joback Method
cpg	869.54	J/molxK	1085.72	Joback Method
cpg	875.87	J/molxK	1124.07	Joback Method
cpg	880.84	J/molxK	1162.42	Joback Method
dvisc	0.0002906	Paxs	574.51	Joback Method

dvisc	0.0001714	Paxs	634.14	Joback Method
dvisc	0.0001107	Paxs	693.78	Joback Method
dvisc	0.0000766	Paxs	753.41	Joback Method
dvisc	0.0000560	Paxs	813.04	Joback Method
dvisc	0.0000427	Paxs	872.68	Joback Method
dvisc	0.0000337	Paxs	932.31	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391875&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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