

Glutaric acid, monochloride, 2-isopropylphenyl ester

Inchi:	InChI=1S/C14H17ClO3/c1-10(2)11-6-3-4-7-12(11)18-14(17)9-5-8-13(15)16/h3-4,6-7,10H
InchiKey:	REFITRWAQBJRDF-UHFFFAOYSA-N
Formula:	C14H17ClO3
SMILES:	CC(C)c1ccccc1OC(=O)CCCC(=O)Cl
Mol. weight [g/mol]:	268.74

Physical Properties

Property code	Value	Unit	Source
gf	-207.43	kJ/mol	Joback Method
hf	-485.63	kJ/mol	Joback Method
hfus	30.73	kJ/mol	Joback Method
hvap	69.60	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	3.651		Crippen Method
mcvol	205.610	ml/mol	McGowan Method
pc	2131.49	kPa	Joback Method
rinpola	1907.00		NIST Webbook
tb	718.53	K	Joback Method
tc	933.24	K	Joback Method
tf	423.49	K	Joback Method
vc	0.784	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	540.43	J/molxK	718.53	Joback Method
cpg	554.31	J/molxK	754.31	Joback Method
cpg	567.25	J/molxK	790.10	Joback Method
cpg	579.26	J/molxK	825.88	Joback Method
cpg	590.38	J/molxK	861.67	Joback Method
cpg	600.62	J/molxK	897.45	Joback Method
cpg	610.02	J/molxK	933.24	Joback Method
dvisc	0.0013717	Paxs	423.49	Joback Method
dvisc	0.0007543	Paxs	472.66	Joback Method

dvisc	0.0004642	Paxs	521.84	Joback Method
dvisc	0.0003106	Paxs	571.01	Joback Method
dvisc	0.0002215	Paxs	620.18	Joback Method
dvisc	0.0001660	Paxs	669.36	Joback Method
dvisc	0.0001295	Paxs	718.53	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358864&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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