

Glutaric acid, 4-chloro-3-methylphenyl ethyl ester

Inchi:	InChI=1S/C14H17ClO4/c1-3-18-13(16)5-4-6-14(17)19-11-7-8-12(15)10(2)9-11/h7-9H,3-6
InchiKey:	VHBJDUWBAKHUJR-UHFFFAOYSA-N
Formula:	C14H17ClO4
SMILES:	CCOC(=O)CCCC(=O)Oc1ccc(Cl)c(C)c1
Mol. weight [g/mol]:	284.74

Physical Properties

Property code	Value	Unit	Source
gf	-319.62	kJ/mol	Joback Method
hf	-624.04	kJ/mol	Joback Method
hfus	35.05	kJ/mol	Joback Method
hvap	73.05	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	3.287		Crippen Method
mcvol	211.480	ml/mol	McGowan Method
pc	2054.89	kPa	Joback Method
rinpola	2105.00		NIST Webbook
rinpola	2105.00		NIST Webbook
tb	746.37	K	Joback Method
tc	956.53	K	Joback Method
tf	473.24	K	Joback Method
vc	0.808	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	564.84	J/molxK	746.37	Joback Method
cpg	621.94	J/molxK	921.51	Joback Method
cpg	612.31	J/molxK	886.48	Joback Method
cpg	601.78	J/molxK	851.45	Joback Method
cpg	590.37	J/molxK	816.42	Joback Method
cpg	578.06	J/molxK	781.40	Joback Method
cpg	630.68	J/molxK	956.53	Joback Method
dvisc	0.0001079	Paxs	746.37	Joback Method

dvisc	0.0001337	Paxs	700.85	Joback Method
dvisc	0.0001708	Paxs	655.33	Joback Method
dvisc	0.0002262	Paxs	609.81	Joback Method
dvisc	0.0003135	Paxs	564.28	Joback Method
dvisc	0.0004601	Paxs	518.76	Joback Method
dvisc	0.0007271	Paxs	473.24	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358790&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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