Glutaric acid, 2-formyl-4-chlorophenyl propyl ester

Other names: Glutaric acid, 2-acetyl-4-chlorophenyl propyl ester
Inchi: InChI=1S/C15H17ClO5/c1-2-8-20-14(18)4-3-5-15(19)21-13-7-6-12(16)9-11(13)10-17/h6-
InchiKey: SZMCCYAMSFSGPN-UHFFFAOYSA-N
Formula: C15H17ClO5
SMILES: CCCOC(=O)CCCC(=O)Oc1ccc(Cl)cc1C=O
Mol. weight [g/mol]: 312.75

Physical Properties

Property code	Value	Unit	Source
gf	-410.72	kJ/mol	Joback Method
hf	-730.26	kJ/mol	Joback Method
hfus	39.93	kJ/mol	Joback Method
hvap	82.00	kJ/mol	Joback Method
log10ws	-4.09		Crippen Method
logp	3.181		Crippen Method
mcvol	227.140	ml/mol	McGowan Method
pc	2014.51	kPa	Joback Method
rinpol	2337.00		NIST Webbook
tb	817.91	K	Joback Method
tc	1029.10	K	Joback Method
tf	526.51	K	Joback Method
vc	0.881	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	631.84	J/mol×K	817.91	Joback Method
cpg	681.38	J/mol×K	993.90	Joback Method
cpg	673.36	J/mol×K	958.70	Joback Method
cpg	664.41	J/mol×K	923.50	Joback Method
cpg	654.51	J/mol×K	888.31	Joback Method
cpg	643.65	J/mol×K	853.11	Joback Method
cpg	688.46	J/mol×K	1029.10	Joback Method
dvisc	0.0001039	Pa×s	817.91	Joback Method

dvisc	0.0001285	Pa×s	769.34	Joback Method
dvisc	0.0001636	Pa×s	720.78	Joback Method
dvisc	0.0002156	Pa×s	672.21	Joback Method
dvisc	0.0002966	Pa×s	623.64	Joback Method
dvisc	0.0004306	Pa×s	575.08	Joback Method
dvisc	0.0006699	Pa×s	526.51	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U358931&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

Latest version available from:
https://www.chemeo.com/cid/33-907-8/Glutaric-acid-2-formyl-4-chlorophenyl-propyl-ester.pdf
Generated by Cheméo on 2024-04-26 13:37:58.060633592 +0000 UTC m=+16427926.981210921.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.