Glutaric acid, 3-chlorophenyl 2-methylhex-3-yl ester

Inchi: InChI=1S/C18H25ClO4/c1-4-7-16(13(2)3)23-18(21)11-6-10-17(20)22-15-9-5-8-14(19)12-

InchiKey: QDPZQWKYQONOQD-UHFFFAOYSA-N

Formula: C18H25ClO4

SMILES: CCCC(OC(=O)CCCC(=O)Oc1cccc(Cl)c1)C(C)C

Mol. weight [g/mol]: 340.84

Physical Properties

Property code	Value	Unit	Source
gf	-281.19	kJ/mol	Joback Method
hf	-705.69	kJ/mol	Joback Method
hfus	38.75	kJ/mol	Joback Method
hvap	80.52	kJ/mol	Joback Method
log10ws	-5.39		Crippen Method
logp	4.784		Crippen Method
mcvol	267.840	ml/mol	McGowan Method
pc	1527.07	kPa	Joback Method
rinpol	2273.00		NIST Webbook
rinpol	2273.00		NIST Webbook
tb	832.03	K	Joback Method
tc	1040.64	K	Joback Method
tf	475.80	K	Joback Method
vc	1.020	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	789.48	J/mol×K	832.03	Joback Method
cpg	852.47	J/mol×K	1005.87	Joback Method
cpg	842.05	J/mol×K	971.10	Joback Method
cpg	830.57	J/mol×K	936.33	Joback Method
cpg	817.99	J/mol×K	901.57	Joback Method
cpg	804.30	J/mol×K	866.80	Joback Method
cpg	861.84	J/mol×K	1040.64	Joback Method
dvisc	0.0000529	Pa×s	832.03	Joback Method

dvisc	0.0000696	Pa×s	772.66	Joback Method
dvisc	0.0000958	Pa×s	713.29	Joback Method
dvisc	0.0001398	Pa×s	653.91	Joback Method
dvisc	0.0002201	Pa×s	594.54	Joback Method
dvisc	0.0003832	Pa×s	535.17	Joback Method
dvisc	0.0007660	Pa×s	475.80	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393756&Units=SI
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

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