Glutaric acid, 2-methylpent-3-yl 4-chloro-2-methoxyphenyl ester

Inchi: InChI=1S/C18H25ClO5/c1-5-14(12(2)3)23-17(20)7-6-8-18(21)24-15-10-9-13(19)11-16(15

InchiKey: SYGNQICWCXKLAF-UHFFFAOYSA-N

Formula: C18H25ClO5

SMILES: CCC(OC(=O)CCCC(=O)Oc1ccc(Cl)cc1OC)C(C)C

Mol. weight [g/mol]: 356.84

Physical Properties

Property code	Value	Unit	Source
gf	-395.82	kJ/mol	Joback Method
hf	-849.38	kJ/mol	Joback Method
hfus	39.55	kJ/mol	Joback Method
hvap	83.59	kJ/mol	Joback Method
log10ws	-5.09		Crippen Method
logp	4.402		Crippen Method
mcvol	273.710	ml/mol	McGowan Method
pc	1489.58	kPa	Joback Method
rinpol	2420.00		NIST Webbook
rinpol	2420.00		NIST Webbook
tb	859.43	K	Joback Method
tc	1068.98	K	Joback Method
tf	510.55	K	Joback Method
vc	1.038	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	816.53	J/mol×K	859.43	Joback Method
cpg	830.72	J/mol×K	894.36	Joback Method
cpg	843.69	J/mol×K	929.28	Joback Method
cpg	855.45	J/mol×K	964.21	Joback Method
cpg	866.00	J/mol×K	999.13	Joback Method
cpg	875.33	J/mol×K	1034.06	Joback Method
cpg	883.46	J/mol×K	1068.98	Joback Method
dvisc	0.0004498	Pa×s	510.55	Joback Method

dvisc	0.0002446	Pa×s	568.70	Joback Method
dvisc	0.0001489	Pa×s	626.84	Joback Method
dvisc	0.0000986	Pa×s	684.99	Joback Method
dvisc	0.0000697	Pa×s	743.14	Joback Method
dvisc	0.0000518	Pa×s	801.28	Joback Method
dvisc	0.0000401	Pa×s	859.43	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393904&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
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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