Glutaric acid, 8-chlorooctyl 4-acetylphenyl ester

Inchi: InChI=1S/C21H29ClO5/c1-17(23)18-11-13-19(14-12-18)27-21(25)10-8-9-20(24)26-16-7-

InchiKey: XHNYYPZCPYUGGA-UHFFFAOYSA-N

Formula: C21H29ClO5

SMILES: CC(=O)c1ccc(OC(=O)CCCC(=O)OCCCCCCCCCCl)cc1

Mol. weight [g/mol]: 396.90

Physical Properties

Property code	Value	Unit	Source
gf	-379.97	kJ/mol	Joback Method
hf	-869.63	kJ/mol	Joback Method
hfus	55.17	kJ/mol	Joback Method
hvap	94.72	kJ/mol	Joback Method
log10ws	-6.07		Crippen Method
logp	5.087		Crippen Method
mcvol	311.680	ml/mol	McGowan Method
pc	1275.51	kPa	Joback Method
rinpol	3165.00		NIST Webbook
rinpol	3165.00		NIST Webbook
tb	955.42	K	Joback Method
tc	1172.11	K	Joback Method
tf	589.54	K	Joback Method
vc	1.206	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	977.30	J/mol×K	955.42	Joback Method
cpg	990.58	J/mol×K	991.54	Joback Method
cpg	1002.57	J/mol×K	1027.65	Joback Method
cpg	1013.31	J/mol×K	1063.77	Joback Method
cpg	1022.82	J/mol×K	1099.88	Joback Method
cpg	1031.15	J/mol×K	1136.00	Joback Method
cpg	1038.31	J/mol×K	1172.11	Joback Method
dvisc	0.0003568	Pa×s	589.54	Joback Method

dvisc	0.0002070	Pa×s	650.52	Joback Method
dvisc	0.0001318	Pa×s	711.50	Joback Method
dvisc	0.0000902	Pa×s	772.48	Joback Method
dvisc	0.0000652	Pa×s	833.46	Joback Method
dvisc	0.0000493	Pa×s	894.44	Joback Method
dvisc	0.0000386	Pa×s	955.42	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392038&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