Glutaric acid, 8-chlorooctyl 4-methoxybenzyl ester

Inchi: InChI=1S/C21H31ClO5/c1-25-19-13-11-18(12-14-19)17-27-21(24)10-8-9-20(23)26-16-7-

InchiKey: VBUFEVSKMSIRTQ-UHFFFAOYSA-N

Formula: C21H31ClO5

SMILES: COc1ccc(COC(=O)CCCC(=O)OCCCCCCCCCl)cc1

Mol. weight [g/mol]: 398.92

Physical Properties

Property code	Value	Unit	Source
gf	-356.05	kJ/mol	Joback Method
hf	-889.27	kJ/mol	Joback Method
hfus	54.76	kJ/mol	Joback Method
hvap	90.38	kJ/mol	Joback Method
log10ws	-5.79		Crippen Method
logp	5.031		Crippen Method
mcvol	315.980	ml/mol	McGowan Method
pc	1205.63	kPa	Joback Method
rinpol	3084.00		NIST Webbook
rinpol	3084.00		NIST Webbook
tb	923.97	K	Joback Method
tc	1133.80	K	Joback Method
tf	561.84	K	Joback Method
vc	1.218	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	992.98	J/mol×K	923.97	Joback Method
cpg	1007.56	J/mol×K	958.94	Joback Method
cpg	1020.81	J/mol×K	993.91	Joback Method
cpg	1032.75	J/mol×K	1028.89	Joback Method
cpg	1043.39	J/mol×K	1063.86	Joback Method
cpg	1052.76	J/mol×K	1098.83	Joback Method
cpg	1060.86	J/mol×K	1133.80	Joback Method
dvisc	0.0003027	Pa×s	561.84	Joback Method

dvisc	0.0001712	Pa×s	622.20	Joback Method
dvisc	0.0001071	Pa×s	682.55	Joback Method
dvisc	0.0000723	Pa×s	742.90	Joback Method
dvisc	0.0000518	Pa×s	803.26	Joback Method
dvisc	0.0000389	Pa×s	863.62	Joback Method
dvisc	0.0000303	Pa×s	923.97	Joback Method

Sources

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=U391748&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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