Glutaric acid, 8-chlorooctyl phenethyl ester

Inchi: InChI=1S/C21H31ClO4/c22-16-8-3-1-2-4-9-17-25-20(23)13-10-14-21(24)26-18-15-19-11
InchiKey: LZNQPHLGZBEKCM-UHFFFAOYSA-N
Formula: C21H31ClO4
SMILES: O=C(CCCC(=O)OCCc1ccccc1)OCCCCCCCCCCl
Mol. weight [g/mol]: 382.92

Physical Properties

Property code	Value	Unit	Source
gf	-241.42	kJ/mol	Joback Method
hf	-745.58	kJ/mol	Joback Method
hfus	53.96	kJ/mol	Joback Method
hvap	87.31	kJ/mol	Joback Method
log10ws	-5.59		Crippen Method
logp	5.065		Crippen Method
mcvol	310.110	ml/mol	McGowan Method
pc	1232.88	kPa	Joback Method
rinpol	2890.00		NIST Webbook
rinpol	2890.00		NIST Webbook
tb	896.57	K	Joback Method
tc	1102.74	K	Joback Method
tf	527.09	K	Joback Method
vc	1.200	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	965.13	J/mol×K	896.57	Joback Method
cpg	980.40	J/mol×K	930.93	Joback Method
cpg	994.48	J/mol×K	965.29	Joback Method
cpg	1007.40	J/mol×K	999.66	Joback Method
cpg	1019.20	J/mol×K	1034.02	Joback Method
cpg	1029.92	J/mol×K	1068.38	Joback Method
cpg	1039.59	J/mol×K	1102.74	Joback Method
dvisc	0.0005010	Pa×s	527.09	Joback Method

dvisc	0.0002640	Pa×s	588.67	Joback Method
dvisc	0.0001570	Pa×s	650.25	Joback Method
dvisc	0.0001022	Pa×s	711.83	Joback Method
dvisc	0.0000712	Pa×s	773.41	Joback Method
dvisc	0.0000523	Pa×s	834.99	Joback Method
dvisc	0.0000401	Pa×s	896.57	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=U391797&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