Glutaric acid, 8-chlorooctyl 5-methyl-2-methoxybenzyl ester

Inchi: InChI=1S/C21H31ClO5/c1-17-12-13-18(25-2)19(16-17)27-21(24)11-9-10-20(23)26-15-8-

InchiKey: BGDDDXDFTDOEQB-UHFFFAOYSA-N

Formula: C21H31ClO5

SMILES: COc1ccc(C)cc1OC(=O)CCCC(=O)OCCCCCCCCCl

Mol. weight [g/mol]: 398.92

Physical Properties

Property code	Value	Unit	Source
gf	-365.68	kJ/mol	Joback Method
hf	-900.74	kJ/mol	Joback Method
hfus	54.37	kJ/mol	Joback Method
hvap	91.05	kJ/mol	Joback Method
log10ws	-6.00		Crippen Method
logp	5.202		Crippen Method
mcvol	315.980	ml/mol	McGowan Method
pc	1193.17	kPa	Joback Method
rinpol	2977.00		NIST Webbook
rinpol	2977.00		NIST Webbook
tb	928.95	K	Joback Method
tc	1139.76	K	Joback Method
tf	574.36	K	Joback Method
vc	1.218	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	992.07	J/mol×K	928.95	Joback Method
cpg	1051.02	J/mol×K	1104.62	Joback Method
cpg	1041.89	J/mol×K	1069.49	Joback Method
cpg	1031.44	J/mol×K	1034.35	Joback Method
cpg	1019.66	J/mol×K	999.22	Joback Method
cpg	1006.54	J/mol×K	964.08	Joback Method
cpg	1058.85	J/mol×K	1139.76	Joback Method
dvisc	0.0000309	Pa×s	928.95	Joback Method

dvisc	0.0000392	Pa×s	869.85	Joback Method
dvisc	0.0000514	Pa×s	810.75	Joback Method
dvisc	0.0000705	Pa×s	751.65	Joback Method
dvisc	0.0001019	Pa×s	692.56	Joback Method
dvisc	0.0001579	Pa×s	633.46	Joback Method
dvisc	0.0002676	Pa×s	574.36	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393932&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