Glutaric acid, 8-chlorooctyl 3-methyl-5-methoxypentyl ester

Inchi: InChI=1S/C20H37ClO5/c1-18(12-16-24-2)13-17-26-20(23)11-9-10-19(22)25-15-8-6-4-3-5

InchiKey: HTTKIYYAIWMMKT-UHFFFAOYSA-N

Formula: C20H37ClO5

SMILES: COCCC(C)CCOC(=O)CCCC(=O)OCCCCCCCCCl

Mol. weight [g/mol]: 392.96

Physical Properties

Property code	Value	Unit	Source
gf	-469.69	kJ/mol	Joback Method
hf	-1098.97	kJ/mol	Joback Method
hfus	54.99	kJ/mol	Joback Method
hvap	84.83	kJ/mol	Joback Method
log10ws	-4.92		Crippen Method
logp	4.885		Crippen Method
mcvol	325.650	ml/mol	McGowan Method
pc	1045.97	kPa	Joback Method
rinpol	2727.00		NIST Webbook
rinpol	2727.00		NIST Webbook
tb	868.99	K	Joback Method
tc	1064.29	K	Joback Method
tf	496.63	K	Joback Method
vc	1.264	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1032.09	J/mol×K	868.99	Joback Method
cpg	1049.17	J/mol×K	901.54	Joback Method
cpg	1065.04	J/mol×K	934.09	Joback Method
cpg	1079.71	J/mol×K	966.64	Joback Method
cpg	1093.17	J/mol×K	999.19	Joback Method
cpg	1105.46	J/mol×K	1031.74	Joback Method
cpg	1116.57	J/mol×K	1064.29	Joback Method
dvisc	0.0005161	Pa×s	496.63	Joback Method

dvisc	0.0002489	Pa×s	558.69	Joback Method
dvisc	0.0001388	Pa×s	620.75	Joback Method
dvisc	0.0000861	Pa×s	682.81	Joback Method
dvisc	0.0000578	Pa×s	744.87	Joback Method
dvisc	0.0000413	Pa×s	806.93	Joback Method
dvisc	0.0000309	Pa×s	868.99	Joback Method

Sources

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=U393530&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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