Glutaric acid, 8-chlorooctyl 2,4-dimethylpent-3-yl ester

Inchi: InChI=1S/C20H37ClO4/c1-16(2)20(17(3)4)25-19(23)13-11-12-18(22)24-15-10-8-6-5-7-9-

InchiKey: ZBZHEFBCOQBFIC-UHFFFAOYSA-N

Formula: C20H37ClO4

SMILES: CC(C)C(OC(=O)CCCC(=O)OCCCCCCCCCCl)C(C)C

Mol. weight [g/mol]: 376.96

Physical Properties

Property code	Value	Unit	Source
gf	-369.57	kJ/mol	Joback Method
hf	-977.31	kJ/mol	Joback Method
hfus	46.76	kJ/mol	Joback Method
hvap	81.65	kJ/mol	Joback Method
log10ws	-5.70		Crippen Method
logp	5.503		Crippen Method
mcvol	319.780	ml/mol	McGowan Method
pc	1068.66	kPa	Joback Method
rinpol	2508.00		NIST Webbook
rinpol	2508.00		NIST Webbook
tb	845.69	K	Joback Method
tc	1038.40	K	Joback Method
tf	444.40	K	Joback Method
vc	1.234	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1002.27	J/mol×K	845.69	Joback Method
cpg	1078.54	J/mol×K	1006.28	Joback Method
cpg	1065.49	J/mol×K	974.16	Joback Method
cpg	1051.36	J/mol×K	942.05	Joback Method
cpg	1036.12	J/mol×K	909.93	Joback Method
cpg	1019.77	J/mol×K	877.81	Joback Method
cpg	1090.53	J/mol×K	1038.40	Joback Method
dvisc	0.0000351	Pa×s	845.69	Joback Method

dvisc	0.0000486	Pa×s	778.81	Joback Method
dvisc	0.0000716	Pa×s	711.93	Joback Method
dvisc	0.0001144	Pa×s	645.05	Joback Method
dvisc	0.0002036	Pa×s	578.16	Joback Method
dvisc	0.0004215	Pa×s	511.28	Joback Method
dvisc	0.0010858	Pa×s	444.40	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=U393484&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