Glutaric acid, hexa-1,5-dien-3-yl 8-chlorooctyl ester

Inchi: InChI=1S/C19H31ClO4/c1-3-12-17(4-2)24-19(22)14-11-13-18(21)23-16-10-8-6-5-7-9-15-

InchiKey: ABMMHYFPVKRFIQ-UHFFFAOYSA-N

Formula: C19H31ClO4

SMILES: C=CCC(C=C)OC(=O)CCCC(=O)OCCCCCCCCCl

Mol. weight [g/mol]: 358.90

Physical Properties

Property code	Value	Unit	Source
gf	-197.43	kJ/mol	Joback Method
hf	-695.25	kJ/mol	Joback Method
hfus	48.65	kJ/mol	Joback Method
hvap	78.86	kJ/mol	Joback Method
log10ws	-5.47		Crippen Method
logp	4.953		Crippen Method
mcvol	297.090	ml/mol	McGowan Method
pc	1193.17	kPa	Joback Method
rinpol	2432.00		NIST Webbook
rinpol	2432.00		NIST Webbook
tb	817.05	K	Joback Method
tc	1006.48	K	Joback Method
tf	459.61	K	Joback Method
vc	1.153	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	887.02	J/mol×K	817.05	Joback Method
cpg	902.97	J/mol×K	848.62	Joback Method
cpg	917.95	J/mol×K	880.19	Joback Method
cpg	931.98	J/mol×K	911.76	Joback Method
cpg	945.09	J/mol×K	943.33	Joback Method
cpg	957.30	J/mol×K	974.90	Joback Method
cpg	968.64	J/mol×K	1006.48	Joback Method
dvisc	0.0008886	Pa×s	459.61	Joback Method

dvisc	0.0004292	Pa×s	519.18	Joback Method
dvisc	0.0002408	Pa×s	578.76	Joback Method
dvisc	0.0001505	Pa×s	638.33	Joback Method
dvisc	0.0001019	Pa×s	697.90	Joback Method
dvisc	0.0000734	Pa×s	757.48	Joback Method
dvisc	0.0000554	Pa×s	817.05	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=U405287&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