Glutaric acid, 3-methylbut-2-en-1-yl 8-chlorooctyl ester

Inchi: InChI=1S/C18H31ClO4/c1-16(2)12-15-23-18(21)11-9-10-17(20)22-14-8-6-4-3-5-7-13-19/

InchiKey: ISGAKJDTIGNMEA-UHFFFAOYSA-N

Formula: C18H31ClO4

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

Mol. weight [g/mol]: 346.89

Physical Properties

Property code	Value	Unit	Source
gf	-307.42	kJ/mol	Joback Method
hf	-812.76	kJ/mol	Joback Method
hfus	51.04	kJ/mol	Joback Method
hvap	78.40	kJ/mol	Joback Method
log10ws	-5.09		Crippen Method
logp	4.789		Crippen Method
mcvol	287.300	ml/mol	McGowan Method
pc	1245.09	kPa	Joback Method
rinpol	2469.00		NIST Webbook
rinpol	2469.00		NIST Webbook
tb	805.29	K	Joback Method
tc	994.25	K	Joback Method
tf	447.82	K	Joback Method
vc	1.121	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	855.33	J/mol×K	805.29	Joback Method
cpg	871.40	J/mol×K	836.78	Joback Method
cpg	886.55	J/mol×K	868.28	Joback Method
cpg	900.80	J/mol×K	899.77	Joback Method
cpg	914.17	J/mol×K	931.26	Joback Method
cpg	926.68	J/mol×K	962.75	Joback Method
cpg	938.37	J/mol×K	994.25	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393461&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

Legend

cpg:	Ideal gas heat capacity
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