Glutaric acid, 3-methylbut-2-en-1-yl octadecyl ester

Inchi: InChI=1S/C28H52O4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-24-31-27(29)21-20
InchiKey: BOJHZNOYNZDTSV-UHFFFAOYSA-N
Formula: C28H52O4
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)CCCC(=O)OCC=C(C)C
Mol. weight [g/mol]: 452.71

Physical Properties

Property code	Value	Unit	Source
gf	-211.29	kJ/mol	Joback Method
hf	-1003.42	kJ/mol	Joback Method
hfus	72.74	kJ/mol	Joback Method
hvap	96.27	kJ/mol	Joback Method
log10ws	-9.12		Crippen Method
logp	8.471		Crippen Method
mcvol	415.960	ml/mol	McGowan Method
pc	708.46	kPa	Joback Method
rinpol	3191.00		NIST Webbook
rinpol	3191.00		NIST Webbook
tb	996.66	K	Joback Method
tc	1232.66	K	Joback Method
tf	530.60	K	Joback Method
vc	1.633	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1446.12	J/mol×K	996.66	Joback Method
cpg	1468.17	J/mol×K	1035.99	Joback Method
cpg	1488.45	J/mol×K	1075.33	Joback Method
cpg	1507.07	J/mol×K	1114.66	Joback Method
cpg	1524.10	J/mol×K	1153.99	Joback Method
cpg	1539.64	J/mol×K	1193.33	Joback Method
cpg	1553.77	J/mol×K	1232.66	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391646&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
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