Glutaric acid, 2,4-dimethylpent-3-yl heptadecyl ester

Inchi: InChI=1S/C29H56O4/c1-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-24-32-27(30)22-21-
InchiKey: LFWJAJOUXMVHKN-UHFFFAOYSA-N
Formula: C29H56O4
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)CCCC(=O)OC(C(C)C)C(C)C
Mol. weight [g/mol]: 468.75

Physical Properties

Property code	Value	Unit	Source
gf	-281.86	kJ/mol	Joback Method
hf	-1147.33	kJ/mol	Joback Method
hfus	65.87	kJ/mol	Joback Method
hvap	97.30	kJ/mol	Joback Method
log10ws	-9.32		Crippen Method
logp	8.795		Crippen Method
mcvol	434.350	ml/mol	McGowan Method
pc	662.21	kPa	Joback Method
rinpol	3185.00		NIST Webbook
tb	1014.18	K	Joback Method
tc	1258.93	K	Joback Method
tf	515.91	K	Joback Method
vc	1.690	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1540.49	J/mol×K	1014.18	Joback Method
cpg	1563.07	J/mol×K	1054.97	Joback Method
cpg	1583.46	J/mol×K	1095.76	Joback Method
cpg	1601.76	J/mol×K	1136.55	Joback Method
cpg	1618.04	J/mol×K	1177.34	Joback Method
cpg	1632.38	J/mol×K	1218.13	Joback Method
cpg	1644.87	J/mol×K	1258.93	Joback Method
dvisc	0.0004111	Pa×s	515.91	Joback Method
dvisc	0.0001445	Pa×s	598.96	Joback Method

dvisc	0.0000655	Pa×s	682.00	Joback Method
dvisc	0.0000353	Pa×s	765.05	Joback Method
dvisc	0.0000214	Pa×s	848.09	Joback Method
dvisc	0.0000142	Pa×s	931.14	Joback Method
dvisc	0.0000101	Pa×s	1014.18	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U359489&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
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