Glutaric acid, trans-hex-3-enyl tridecyl ester

Inchi: InChI=1S/C24H44O4/c1-3-5-7-9-10-11-12-13-14-15-17-22-28-24(26)20-18-19-23(25)27-
InchiKey: FKXYPIIZXAKLGR-SOFGYWHQSA-N
Formula: C24H44O4
SMILES: CCC=CCCOC(=O)CCCC(=O)OCCCCCCCCCCCCC
Mol. weight [g/mol]: 396.60

Physical Properties

Property code	Value	Unit	Source
gf	-236.42	kJ/mol	Joback Method
hf	-911.07	kJ/mol	Joback Method
hfus	63.69	kJ/mol	Joback Method
hvap	87.29	kJ/mol	Joback Method
log10ws	-7.45		Crippen Method
logp	6.910		Crippen Method
mcvol	359.600	ml/mol	McGowan Method
pc	876.36	kPa	Joback Method
rinpol	2792.00		NIST Webbook
tb	905.26	K	Joback Method
tc	1108.91	K	Joback Method
tf	499.48	K	Joback Method
vc	1.407	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1190.55	J/mol×K	905.26	Joback Method
cpg	1275.94	J/mol×K	1074.97	Joback Method
cpg	1261.26	J/mol×K	1041.03	Joback Method
cpg	1245.42	J/mol×K	1007.08	Joback Method
cpg	1228.39	J/mol×K	973.14	Joback Method
cpg	1210.11	J/mol×K	939.20	Joback Method
cpg	1289.52	J/mol×K	1108.91	Joback Method
dvisc	0.0000257	Pa×s	905.26	Joback Method
dvisc	0.0000345	Pa×s	837.63	Joback Method

dvisc	0.0000486	Pa×s	770.00	Joback Method
dvisc	0.0000733	Pa×s	702.37	Joback Method
dvisc	0.0001206	Pa×s	634.74	Joback Method
dvisc	0.0002235	Pa×s	567.11	Joback Method
dvisc	0.0004895	Pa×s	499.48	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=U359933&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

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