Glutaric acid, di(1-(cyclohex-2-enyl)hex-3-yl) ester

Inchi: InChI=1S/C29H48O4/c1-3-12-26(22-20-24-14-7-5-8-15-24)32-28(30)18-11-19-29(31)33-

InchiKey: MLGJUOQVXOIHTH-UHFFFAOYSA-N

Formula: C29H48O4

SMILES: CCCC(CCC1C=CCCC1)OC(=O)CCCC(=O)OC(CCC)CCC1C=CCCC1

Mol. weight [g/mol]: 460.69

Physical Properties

Property code	Value	Unit	Source
gf	-170.60	kJ/mol	Joback Method
hf	-917.85	kJ/mol	Joback Method
hfus	55.51	kJ/mol	Joback Method
hvap	99.13	kJ/mol	Joback Method
log10ws	-8.92		Crippen Method
logp	7.853		Crippen Method
mcvol	404.030	ml/mol	McGowan Method
pc	858.98	kPa	Joback Method
rinpol	3145.00		NIST Webbook
rinpol	3145.00		NIST Webbook
tb	1052.04	K	Joback Method
tc	1288.27	K	Joback Method
tf	547.19	K	Joback Method
vc	1.534	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1465.48	J/mol×K	1052.04	Joback Method
cpg	1482.88	J/mol×K	1091.41	Joback Method
cpg	1498.18	J/mol×K	1130.78	Joback Method
cpg	1511.48	J/mol×K	1170.15	Joback Method
cpg	1522.85	J/mol×K	1209.52	Joback Method
cpg	1532.39	J/mol×K	1248.90	Joback Method
cpg	1540.18	J/mol×K	1288.27	Joback Method
dvisc	0.0004342	Pa×s	547.19	Joback Method

dvisc	0.0001675	Pa×s	631.33	Joback Method
dvisc	0.0000808	Pa×s	715.47	Joback Method
dvisc	0.0000455	Pa×s	799.62	Joback Method
dvisc	0.0000286	Pa×s	883.76	Joback Method
dvisc	0.0000194	Pa×s	967.90	Joback Method
dvisc	0.0000141	Pa×s	1052.04	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405519&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

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