

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
mvol	404.030	ml/mol	McGowan Method
pc	858.98	kPa	Joback Method
rinpol	3145.00		NIST Webbook
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tb	1052.04	K	Joback Method
tc	1288.27	K	Joback Method
tf	547.19	K	Joback Method
vc	1.534	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0001675	Paxs	631.33	Joback Method
dvisc	0.0000808	Paxs	715.47	Joback Method
dvisc	0.0000455	Paxs	799.62	Joback Method
dvisc	0.0000286	Paxs	883.76	Joback Method
dvisc	0.0000194	Paxs	967.90	Joback Method
dvisc	0.0000141	Paxs	1052.04	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U405519&Units=SI

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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