Glutaric acid, hex-4-en-1-yl cyclohexylmethyl ester

Inchi: InChI=1S/C18H30O4/c1-2-3-4-8-14-21-17(19)12-9-13-18(20)22-15-16-10-6-5-7-11-16/h2

InchiKey: GRVUWOHDHJZHDS-NSCUHMNNSA-N

Formula: C18H30O4

SMILES: CC=CCCCOC(=O)CCCC(=O)OCC1CCCCC1

Mol. weight [g/mol]: 310.43

Physical Properties

Property code	Value	Unit	Source
gf	-262.49	kJ/mol	Joback Method
hf	-732.91	kJ/mol	Joback Method
hfus	39.99	kJ/mol	Joback Method
hvap	74.36	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	4.180		Crippen Method
mcvol	264.200	ml/mol	McGowan Method
pc	1482.71	kPa	Joback Method
rinpol	2247.00		NIST Webbook
rinpol	2247.00		NIST Webbook
tb	787.53	K	Joback Method
tc	987.34	K	Joback Method
tf	439.24	K	Joback Method
vc	1.004	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	821.16	J/mol×K	787.53	Joback Method
cpg	900.47	J/mol×K	954.04	Joback Method
cpg	886.86	J/mol×K	920.74	Joback Method
cpg	872.16	J/mol×K	887.44	Joback Method
cpg	856.33	J/mol×K	854.13	Joback Method
cpg	839.34	J/mol×K	820.83	Joback Method
cpg	913.01	J/mol×K	987.34	Joback Method
dvisc	0.0000637	Pa×s	787.53	Joback Method

dvisc	0.0000849	Pa×s	729.48	Joback Method
dvisc	0.0001188	Pa×s	671.43	Joback Method
dvisc	0.0001774	Pa×s	613.38	Joback Method
dvisc	0.0002880	Pa×s	555.34	Joback Method
dvisc	0.0005234	Pa×s	497.29	Joback Method
dvisc	0.0011139	Pa×s	439.24	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405303&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

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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