Glutaric acid, pent-2-en-1-yl cyclohexylmethyl ester

Inchi: InChI=1S/C17H28O4/c1-2-3-7-13-20-16(18)11-8-12-17(19)21-14-15-9-5-4-6-10-15/h3,7,
InchiKey: GPABDNZRDCKSTQ-XVNBXDOJSA-N
Formula: C17H28O4
SMILES: CCC=CCOC(=O)CCCC(=O)OCC1CCCCC1
Mol. weight [g/mol]: 296.40

Physical Properties

Property code	Value	Unit	Source
gf	-270.91	kJ/mol	Joback Method
hf	-712.27	kJ/mol	Joback Method
hfus	37.40	kJ/mol	Joback Method
hvap	72.13	kJ/mol	Joback Method
log10ws	-4.17		Crippen Method
logp	3.790		Crippen Method
mcvol	250.110	ml/mol	McGowan Method
pc	1598.72	kPa	Joback Method
rinpol	2152.00		NIST Webbook
rinpol	2152.00		NIST Webbook
tb	764.65	K	Joback Method
tc	965.43	K	Joback Method
tf	427.97	K	Joback Method
vc	0.949	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	762.73	J/mol×K	764.65	Joback Method
cpg	841.56	J/mol×K	931.97	Joback Method
cpg	828.01	J/mol×K	898.50	Joback Method
cpg	813.37	J/mol×K	865.04	Joback Method
cpg	797.63	J/mol×K	831.58	Joback Method
cpg	780.76	J/mol×K	798.11	Joback Method
cpg	854.06	J/mol×K	965.43	Joback Method
dvisc	0.0000731	Pa×s	764.65	Joback Method

dvisc	0.0000971	Pa×s	708.54	Joback Method
dvisc	0.0001356	Pa×s	652.42	Joback Method
dvisc	0.0002015	Pa×s	596.31	Joback Method
dvisc	0.0003253	Pa×s	540.20	Joback Method
dvisc	0.0005866	Pa×s	484.08	Joback Method
dvisc	0.0012350	Pa×s	427.97	Joback Method

Sources

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=U405259&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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