Glutaric acid, hept-2-yl but-3-en-1-yl ester

Inchi: InChI=1S/C16H28O4/c1-4-6-8-10-14(3)20-16(18)12-9-11-15(17)19-13-7-5-2/h5,14H,2,4,
InchiKey: GHYSGUSPYYJFSL-UHFFFAOYSA-N
Formula: C16H28O4
SMILES: C=CCCOC(=O)CCCC(=O)OC(C)CCCCC
Mol. weight [g/mol]: 284.39

Physical Properties

Property code	Value	Unit	Source
gf	-298.60	kJ/mol	Joback Method
hf	-743.02	kJ/mol	Joback Method
hfus	37.97	kJ/mol	Joback Method
hvap	68.46	kJ/mol	Joback Method
log10ws	-4.21		Crippen Method
logp	3.788		Crippen Method
mcvol	246.880	ml/mol	McGowan Method
pc	1465.73	kPa	Joback Method
rinpol	1943.00		NIST Webbook
rinpol	1943.00		NIST Webbook
tb	714.30	K	Joback Method
tc	894.16	K	Joback Method
tf	397.64	K	Joback Method
vc	0.955	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	709.52	J/mol×K	714.30	Joback Method
cpg	725.77	J/mol×K	744.28	Joback Method
cpg	741.19	J/mol×K	774.25	Joback Method
cpg	755.79	J/mol×K	804.23	Joback Method
cpg	769.59	J/mol×K	834.21	Joback Method
cpg	782.59	J/mol×K	864.18	Joback Method
cpg	794.81	J/mol×K	894.16	Joback Method
dvisc	0.0015131	Pa×s	397.64	Joback Method

dvisc	0.0007187	Pa×s	450.42	Joback Method
dvisc	0.0003991	Pa×s	503.19	Joback Method
dvisc	0.0002478	Pa×s	555.97	Joback Method
dvisc	0.0001671	Pa×s	608.75	Joback Method
dvisc	0.0001200	Pa×s	661.52	Joback Method
dvisc	0.0000905	Pa×s	714.30	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U394036&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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