Glutaric acid, hexa-1,5-dien-3-yl hept-2-yl ester

Inchi: InChI=1S/C18H30O4/c1-5-8-9-12-15(4)21-17(19)13-10-14-18(20)22-16(7-3)11-6-2/h6-7,
InchiKey: FJDNFFNUHAKPIH-UHFFFAOYSA-N
Formula: C18H30O4
SMILES: C=CCC(C=C)OC(=O)CCCC(=O)OC(C)CCCCC
Mol. weight [g/mol]: 310.43

Physical Properties

Property code	Value	Unit	Source
gf	-196.36	kJ/mol	Joback Method
hf	-664.15	kJ/mol	Joback Method
hfus	38.34	kJ/mol	Joback Method
hvap	71.86	kJ/mol	Joback Method
log10ws	-5.01		Crippen Method
logp	4.343		Crippen Method
mcvol	270.760	ml/mol	McGowan Method
pc	1318.48	kPa	Joback Method
rinpol	1910.00		NIST Webbook
rinpol	1910.00		NIST Webbook
tb	756.30	K	Joback Method
tc	940.44	K	Joback Method
tf	403.42	K	Joback Method
vc	1.042	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	799.04	J/mol×K	756.30	Joback Method
cpg	815.72	J/mol×K	786.99	Joback Method
cpg	831.48	J/mol×K	817.68	Joback Method
cpg	846.33	J/mol×K	848.37	Joback Method
cpg	860.29	J/mol×K	879.06	Joback Method
cpg	873.39	J/mol×K	909.75	Joback Method
cpg	885.64	J/mol×K	940.44	Joback Method
dvisc	0.0015140	Pa×s	403.42	Joback Method

dvisc	0.0006487	Pa×s	462.23	Joback Method
dvisc	0.0003366	Pa×s	521.05	Joback Method
dvisc	0.0001995	Pa×s	579.86	Joback Method
dvisc	0.0001302	Pa×s	638.67	Joback Method
dvisc	0.0000913	Pa×s	697.49	Joback Method
dvisc	0.0000677	Pa×s	756.30	Joback Method

Sources

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=U405279&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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