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

Inchi: InChI=1S/C16H26O4/c1-6-9-14(7-2)20-16(18)11-8-10-15(17)19-13(5)12(3)4/h6-7,12-14H

InchiKey: CQDDWSWNJBSPNN-UHFFFAOYSA-N

Formula: C16H26O4

SMILES: C=CCC(C=C)OC(=O)CCCC(=O)OC(C)C(C)C

Mol. weight [g/mol]: 282.38

Physical Properties

Property code	Value	Unit	Source
gf	-215.64	kJ/mol	Joback Method
hf	-628.15	kJ/mol	Joback Method
hfus	29.64	kJ/mol	Joback Method
hvap	67.02	kJ/mol	Joback Method
log10ws	-3.93		Crippen Method
logp	3.418		Crippen Method
mcvol	242.580	ml/mol	McGowan Method
pc	1533.06	kPa	Joback Method
rinpol	1713.00		NIST Webbook
rinpol	1713.00		NIST Webbook
tb	710.10	K	Joback Method
tc	896.56	K	Joback Method
tf	365.88	K	Joback Method
vc	0.923	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	686.11	J/mol×K	710.10	Joback Method
cpg	702.29	J/mol×K	741.18	Joback Method
cpg	717.59	J/mol×K	772.25	Joback Method
cpg	732.03	J/mol×K	803.33	Joback Method
cpg	745.62	J/mol×K	834.40	Joback Method
cpg	758.39	J/mol×K	865.48	Joback Method
cpg	770.33	J/mol×K	896.56	Joback Method
dvisc	0.0023541	Pa×s	365.88	Joback Method

dvisc	0.0009198	Pa×s	423.25	Joback Method
dvisc	0.0004498	Pa×s	480.62	Joback Method
dvisc	0.0002562	Pa×s	537.99	Joback Method
dvisc	0.0001626	Pa×s	595.36	Joback Method
dvisc	0.0001118	Pa×s	652.73	Joback Method
dvisc	0.0000817	Pa×s	710.10	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405275&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