Glutaric acid, hexa-1,5-dien-3-yl cyclohexylmethyl ester

Inchi: InChI=1S/C18H28O4/c1-3-9-16(4-2)22-18(20)13-8-12-17(19)21-14-15-10-6-5-7-11-15/h3

InchiKey: AUPQGTKDTVLKTM-UHFFFAOYSA-N

Formula: C18H28O4

SMILES: C=CCC(C=C)OC(=O)CCCC(=O)OCC1CCCCC1

Mol. weight [g/mol]: 308.41

Physical Properties

Property code	Value	Unit	Source
gf	-169.47	kJ/mol	Joback Method
hf	-604.55	kJ/mol	Joback Method
hfus	33.70	kJ/mol	Joback Method
hvap	72.67	kJ/mol	Joback Method
log10ws	-4.55		Crippen Method
logp	3.954		Crippen Method
mcvol	259.900	ml/mol	McGowan Method
pc	1529.46	kPa	Joback Method
rinpol	2105.00		NIST Webbook
rinpol	2105.00		NIST Webbook
tb	776.29	K	Joback Method
tc	977.84	K	Joback Method
tf	425.80	K	Joback Method
vc	0.981	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	794.10	J/mol×K	776.29	Joback Method
cpg	872.00	J/mol×K	944.25	Joback Method
cpg	858.73	J/mol×K	910.66	Joback Method
cpg	844.33	J/mol×K	877.06	Joback Method
cpg	828.78	J/mol×K	843.47	Joback Method
cpg	812.05	J/mol×K	809.88	Joback Method
cpg	884.16	J/mol×K	977.84	Joback Method
dvisc	0.0000765	Pa×s	776.29	Joback Method

dvisc	0.0001023	Pa×s	717.88	Joback Method
dvisc	0.0001440	Pa×s	659.46	Joback Method
dvisc	0.0002167	Pa×s	601.04	Joback Method
dvisc	0.0003562	Pa×s	542.63	Joback Method
dvisc	0.0006599	Pa×s	484.21	Joback Method
dvisc	0.0014480	Pa×s	425.80	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405282&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