

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

Inchi: InChI=1S/C21H36O4/c1-5-8-9-10-11-12-15-18(4)24-20(22)16-13-17-21(23)25-19(7-3)14
InchiKey: ZMUXMDKSSHQVIH-UHFFFAOYSA-N
Formula: C21H36O4
SMILES: C=CCC(C=C)OC(=O)CCCC(=O)OC(C)CCCCCCCC
Mol. weight [g/mol]: 352.51

Physical Properties

Property code	Value	Unit	Source
gf	-171.10	kJ/mol	Joback Method
hf	-726.07	kJ/mol	Joback Method
hfus	46.11	kJ/mol	Joback Method
hvap	78.54	kJ/mol	Joback Method
log10ws	-6.27		Crippen Method
logp	5.513		Crippen Method
mcvol	313.030	ml/mol	McGowan Method
pc	1080.64	kPa	Joback Method
rinpol	2204.00		NIST Webbook
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tb	824.94	K	Joback Method
tc	1013.79	K	Joback Method
tf	437.23	K	Joback Method
vc	1.210	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	976.43	J/molxK	824.94	Joback Method
cpg	994.15	J/molxK	856.42	Joback Method
cpg	1010.80	J/molxK	887.89	Joback Method
cpg	1026.41	J/molxK	919.37	Joback Method
cpg	1041.00	J/molxK	950.84	Joback Method
cpg	1054.61	J/molxK	982.32	Joback Method
cpg	1067.26	J/molxK	1013.79	Joback Method
dvisc	0.0010788	Paxs	437.23	Joback Method

dvisc	0.0004499	Paxs	501.85	Joback Method
dvisc	0.0002291	Paxs	566.47	Joback Method
dvisc	0.0001339	Paxs	631.09	Joback Method
dvisc	0.0000865	Paxs	695.70	Joback Method
dvisc	0.0000602	Paxs	760.32	Joback Method
dvisc	0.0000443	Paxs	824.94	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U405285&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

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