

Glutaric acid, oct-1-en-3-yl 2-ethylhexyl ester

Inchi: InChI=1S/C21H38O4/c1-5-9-11-14-19(8-4)25-21(23)16-12-15-20(22)24-17-18(7-3)13-10
InchiKey: SOHLTFSLOBUHRA-UHFFFAOYSA-N
Formula: C21H38O4
SMILES: C=CC(CCCCC)OC(=O)CCCC(=O)OCC(CC)CCCC
Mol. weight [g/mol]: 354.52

Physical Properties

Property code	Value	Unit	Source
gf	-258.94	kJ/mol	Joback Method
hf	-851.50	kJ/mol	Joback Method
hfus	47.39	kJ/mol	Joback Method
hvap	79.21	kJ/mol	Joback Method
log10ws	-6.06		Crippen Method
logp	5.594		Crippen Method
mvol	317.330	ml/mol	McGowan Method
pc	1051.41	kPa	Joback Method
rinpol	2231.00		NIST Webbook
rinpol	2231.00		NIST Webbook
tb	828.26	K	Joback Method
tc	1016.75	K	Joback Method
tf	438.99	K	Joback Method
vc	1.228	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1003.75	J/molxK	828.26	Joback Method
cpg	1084.17	J/molxK	985.33	Joback Method
cpg	1070.20	J/molxK	953.92	Joback Method
cpg	1055.20	J/molxK	922.50	Joback Method
cpg	1039.14	J/molxK	891.09	Joback Method
cpg	1021.99	J/molxK	859.67	Joback Method
cpg	1097.13	J/molxK	1016.75	Joback Method
dvisc	0.0000414	Paxs	828.26	Joback Method

dvisc	0.0000566	Paxs	763.38	Joback Method
dvisc	0.0000819	Paxs	698.50	Joback Method
dvisc	0.0001277	Paxs	633.62	Joback Method
dvisc	0.0002206	Paxs	568.75	Joback Method
dvisc	0.0004385	Paxs	503.87	Joback Method
dvisc	0.0010680	Paxs	438.99	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=U405352&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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