

Glutaric acid, but-3-en-2-yl dodec-2-en-1-yl ester

Inchi:	InChI=1S/C21H36O4/c1-4-6-7-8-9-10-11-12-13-14-18-24-20(22)16-15-17-21(23)25-19(3)
InchiKey:	VWHMBRMQYHRSRX-BUHFOSPRSA-N
Formula:	C21H36O4
SMILES:	C=CC(C)OC(=O)CCCC(=O)OCC=CCCCCCCCC
Mol. weight [g/mol]:	352.51

Physical Properties

Property code	Value	Unit	Source
gf	-176.28	kJ/mol	Joback Method
hf	-729.00	kJ/mol	Joback Method
hfus	51.12	kJ/mol	Joback Method
hvap	79.55	kJ/mol	Joback Method
log10ws	-6.16		Crippen Method
logp	5.514		Crippen Method
mvol	313.030	ml/mol	McGowan Method
pc	1082.06	kPa	Joback Method
rinpol	2361.00		NIST Webbook
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tb	832.86	K	Joback Method
tc	1022.98	K	Joback Method
tf	448.91	K	Joback Method
vc	1.214	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	977.48	J/molxK	832.86	Joback Method
cpg	1055.62	J/molxK	991.29	Joback Method
cpg	1041.92	J/molxK	959.60	Joback Method
cpg	1027.29	J/molxK	927.92	Joback Method
cpg	1011.70	J/molxK	896.23	Joback Method
cpg	995.11	J/molxK	864.55	Joback Method
cpg	1068.41	J/molxK	1022.98	Joback Method
dvisc	0.0000394	Paxs	832.86	Joback Method

dvisc	0.0000530	Paxs	768.87	Joback Method
dvisc	0.0000752	Paxs	704.88	Joback Method
dvisc	0.0001147	Paxs	640.88	Joback Method
dvisc	0.0001918	Paxs	576.89	Joback Method
dvisc	0.0003649	Paxs	512.90	Joback Method
dvisc	0.0008337	Paxs	448.91	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=U405247&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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