

Glutaric acid, dodec-2-en-1-yl 3-methyl-5-methoxypentyl ester

Inchi:	InChI=1S/C24H44O5/c1-4-5-6-7-8-9-10-11-12-13-19-28-23(25)15-14-16-24(26)29-21-18
InchiKey:	NPXBTPDBTHHWPK-OUKQBFOZSA-N
Formula:	C24H44O5
SMILES:	CCCCCCCCC=CCOC(=O)CCCC(=O)OCCC(C)CCOC
Mol. weight [g/mol]:	412.60

Physical Properties

Property code	Value	Unit	Source
gf	-343.86	kJ/mol	Joback Method
hf	-1048.57	kJ/mol	Joback Method
hfus	61.36	kJ/mol	Joback Method
hvap	89.31	kJ/mol	Joback Method
log10ws	-6.29		Crippen Method
logp	6.003		Crippen Method
mcvol	365.470	ml/mol	McGowan Method
pc	871.71	kPa	Joback Method
rinqol	2805.00		NIST Webbook
tb	927.24	K	Joback Method
tc	1136.52	K	Joback Method
tf	506.71	K	Joback Method
vc	1.419	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1222.67	J/molxK	927.24	Joback Method
cpg	1241.84	J/molxK	962.12	Joback Method
cpg	1259.55	J/molxK	997.00	Joback Method
cpg	1275.84	J/molxK	1031.88	Joback Method
cpg	1290.75	J/molxK	1066.76	Joback Method
cpg	1304.32	J/molxK	1101.64	Joback Method
cpg	1316.56	J/molxK	1136.52	Joback Method
dvisc	0.0003780	Paxs	506.71	Joback Method
dvisc	0.0001655	Paxs	576.80	Joback Method

dvisc	0.0000867	Paxs	646.89	Joback Method
dvisc	0.0000515	Paxs	716.97	Joback Method
dvisc	0.0000336	Paxs	787.06	Joback Method
dvisc	0.0000235	Paxs	857.15	Joback Method
dvisc	0.0000173	Paxs	927.24	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=U393532&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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