

Glutaric acid, dodec-2-en-1-yl 2,4,4-trimethylpentyl ester

Inchi:	InChI=1S/C25H46O4/c1-6-7-8-9-10-11-12-13-14-15-19-28-23(26)17-16-18-24(27)29-21-
InchiKey:	QTVGSZSMUOEABJ-CCEZHUSRSA-N
Formula:	C25H46O4
SMILES:	CCCCCCCCC=CCOC(=O)CCCC(=O)OCC(C)CC(C)(C)C
Mol. weight [g/mol]:	410.63

Physical Properties

Property code	Value	Unit	Source
gf	-227.60	kJ/mol	Joback Method
hf	-945.74	kJ/mol	Joback Method
hfus	55.34	kJ/mol	Joback Method
hvap	87.83	kJ/mol	Joback Method
log10ws	-7.38		Crippen Method
logp	7.012		Crippen Method
mvol	373.690	ml/mol	McGowan Method
pc	841.62	kPa	Joback Method
rinpol	2706.00		NIST Webbook
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tb	924.47	K	Joback Method
tc	1131.98	K	Joback Method
tf	498.17	K	Joback Method
vc	1.446	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1254.11	J/molxK	924.47	Joback Method
cpg	1273.85	J/molxK	959.06	Joback Method
cpg	1292.30	J/molxK	993.64	Joback Method
cpg	1309.54	J/molxK	1028.23	Joback Method
cpg	1325.63	J/molxK	1062.81	Joback Method
cpg	1340.65	J/molxK	1097.40	Joback Method
cpg	1354.65	J/molxK	1131.98	Joback Method
dvisc	0.0004577	Paxs	498.17	Joback Method

dvisc	0.0001832	Paxs	569.22	Joback Method
dvisc	0.0000898	Paxs	640.27	Joback Method
dvisc	0.0000508	Paxs	711.32	Joback Method
dvisc	0.0000318	Paxs	782.37	Joback Method
dvisc	0.0000216	Paxs	853.42	Joback Method
dvisc	0.0000155	Paxs	924.47	Joback Method

Sources

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=U391542&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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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