

Glutaric acid, dec-2-yl 3,7-dimethyloctyl ester

Inchi: InChI=1S/C25H48O4/c1-6-7-8-9-10-11-16-23(5)29-25(27)18-13-17-24(26)28-20-19-22(4)
InchiKey: VDFNXPDSFWFNRS-UHFFFAOYSA-N
Formula: C25H48O4
SMILES: CCCCCCCC(C)OC(=O)CCCC(=O)OCCC(C)CCCC(C)C
Mol. weight [g/mol]: 412.65

Physical Properties

Property code	Value	Unit	Source
gf	-315.54	kJ/mol	Joback Method
hf	-1064.77	kJ/mol	Joback Method
hfus	55.51	kJ/mol	Joback Method
hvap	88.39	kJ/mol	Joback Method
log10ws	-7.64		Crippen Method
logp	7.235		Crippen Method
mcvol	377.990	ml/mol	McGowan Method
pc	815.39	kPa	Joback Method
rinpol	2611.00		NIST Webbook
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tb	922.66	K	Joback Method
tc	1130.87	K	Joback Method
tf	470.83	K	Joback Method
vc	1.466	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1282.35	J/molxK	922.66	Joback Method
cpg	1302.76	J/molxK	957.36	Joback Method
cpg	1321.65	J/molxK	992.06	Joback Method
cpg	1339.04	J/molxK	1026.76	Joback Method
cpg	1354.98	J/molxK	1061.46	Joback Method
cpg	1369.52	J/molxK	1096.16	Joback Method
cpg	1382.68	J/molxK	1130.87	Joback Method
dvisc	0.0007421	Paxs	470.83	Joback Method

dvisc	0.0002651	Paxs	546.13	Joback Method
dvisc	0.0001216	Paxs	621.44	Joback Method
dvisc	0.0000660	Paxs	696.75	Joback Method
dvisc	0.0000403	Paxs	772.05	Joback Method
dvisc	0.0000269	Paxs	847.36	Joback Method
dvisc	0.0000192	Paxs	922.66	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=U391488&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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