Glutaric acid, dodecyl 3-oxobut-2-yl ester

Inchi: InChI=1S/C21H38O5/c1-4-5-6-7-8-9-10-11-12-13-17-25-20(23)15-14-16-21(24)26-19(3)1
InchiKey: HTPLGYMFFHWKAA-UHFFFAOYSA-N
Formula: C21H38O5
SMILES: CCCCCCCCCCCCOC(=O)CCCC(=O)OC(C)C(C)=O
Mol. weight [g/mol]: 370.52

Physical Properties

Property code	Value	Unit	Source
gf	-473.26	kJ/mol	Joback Method
hf	-1084.23	kJ/mol	Joback Method
hfus	53.80	kJ/mol	Joback Method
hvap	87.01	kJ/mol	Joback Method
log10ws	-5.73		Crippen Method
logp	5.141		Crippen Method
mcvol	323.200	ml/mol	McGowan Method
pc	1060.33	kPa	Joback Method
rinpol	2587.00		NIST Webbook
tb	885.89	K	Joback Method
tc	1084.76	K	Joback Method
tf	505.68	K	Joback Method
vc	1.260	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1053.22	J/mol×K	885.89	Joback Method
cpg	1127.14	J/mol×K	1051.61	Joback Method
cpg	1114.75	J/mol×K	1018.47	Joback Method
cpg	1101.18	J/mol×K	985.32	Joback Method
cpg	1086.42	J/mol×K	952.18	Joback Method
cpg	1070.44	J/mol×K	919.03	Joback Method
cpg	1138.39	J/mol×K	1084.76	Joback Method
dvisc	0.0000398	Pa×s	885.89	Joback Method
dvisc	0.0000531	Pa×s	822.52	Joback Method

dvisc	0.0000743	Pa×s	759.15	Joback Method
dvisc	0.0001105	Pa×s	695.78	Joback Method
dvisc	0.0001780	Pa×s	632.42	Joback Method
dvisc	0.0003187	Pa×s	569.05	Joback Method
dvisc	0.0006604	Pa×s	505.68	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359712&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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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