Glutaric acid, 2-methylpent-3-yl 2,4-dimethylpent-3-yl ester

Inchi: InChI=1S/C18H34O4/c1-8-15(12(2)3)21-16(19)10-9-11-17(20)22-18(13(4)5)14(6)7/h12-1

InchiKey: IYTSMQCIDJTVKH-UHFFFAOYSA-N

Formula: C18H34O4

SMILES: CCC(OC(=O)CCCC(=O)OC(C(C)C)C(C)C)C(C)C

Mol. weight [g/mol]: 314.46

Physical Properties

Property code	Value	Unit	Source
gf	-379.36	kJ/mol	Joback Method
hf	-930.85	kJ/mol	Joback Method
hfus	30.34	kJ/mol	Joback Method
hvap	72.03	kJ/mol	Joback Method
log10ws	-4.58		Crippen Method
logp	4.358		Crippen Method
mcvol	279.360	ml/mol	McGowan Method
pc	1262.85	kPa	Joback Method
rinpol	1860.00		NIST Webbook
rinpol	1860.00		NIST Webbook
tb	761.62	K	Joback Method
tc	948.22	K	Joback Method
tf	361.94	K	Joback Method
vc	1.062	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	851.92	J/mol×K	761.62	Joback Method
cpg	870.15	J/mol×K	792.72	Joback Method
cpg	887.34	J/mol×K	823.82	Joback Method
cpg	903.51	J/mol×K	854.92	Joback Method
cpg	918.65	J/mol×K	886.02	Joback Method
cpg	932.80	J/mol×K	917.12	Joback Method
cpg	945.95	J/mol×K	948.22	Joback Method
dvisc	0.0032825	Pa×s	361.94	Joback Method

dvisc	0.0009323	Pa×s	428.55	Joback Method
dvisc	0.0003715	Pa×s	495.17	Joback Method
dvisc	0.0001841	Pa×s	561.78	Joback Method
dvisc	0.0001059	Pa×s	628.39	Joback Method
dvisc	0.0000677	Pa×s	695.01	Joback Method
dvisc	0.0000468	Pa×s	761.62	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393474&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