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

Inchi: InChI=1S/C18H34O4/c1-13(2)9-8-12-21-16(19)10-7-11-17(20)22-18(14(3)4)15(5)6/h13-1
InchiKey: XXHQQGXDOCDUKX-UHFFFAOYSA-N
Formula: C18H34O4
SMILES: CC(C)CCCOC(=O)CCCC(=O)OC(C(C)C)C(C)C
Mol. weight [g/mol]: 314.46

Physical Properties

Property code	Value	Unit	Source
gf	-376.92	kJ/mol	Joback Method
hf	-925.57	kJ/mol	Joback Method
hfus	33.86	kJ/mol	Joback Method
hvap	72.42	kJ/mol	Joback Method
log10ws	-4.47		Crippen Method
logp	4.360		Crippen Method
mcvol	279.360	ml/mol	McGowan Method
pc	1255.70	kPa	Joback Method
rinpol	2011.00		NIST Webbook
rinpol	2011.00		NIST Webbook
tb	762.06	K	Joback Method
tc	946.82	K	Joback Method
tf	376.94	K	Joback Method
vc	1.067	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	851.43	J/mol×K	762.06	Joback Method
cpg	869.48	J/mol×K	792.85	Joback Method
cpg	886.51	J/mol×K	823.65	Joback Method
cpg	902.54	J/mol×K	854.44	Joback Method
cpg	917.58	J/mol×K	885.24	Joback Method
cpg	931.65	J/mol×K	916.03	Joback Method
cpg	944.75	J/mol×K	946.82	Joback Method
dvisc	0.0024596	Pa×s	376.94	Joback Method

dvisc	0.0008051	Pa×s	441.13	Joback Method
dvisc	0.0003500	Pa×s	505.31	Joback Method
dvisc	0.0001836	Pa×s	569.50	Joback Method
dvisc	0.0001097	Pa×s	633.69	Joback Method
dvisc	0.0000721	Pa×s	697.87	Joback Method
dvisc	0.0000509	Pa×s	762.06	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359477&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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