

Glutaric acid, 2-methylpent-3-yl 2-methylhex-3-yl ester

Inchi:	InChI=1S/C18H34O4/c1-7-10-16(14(5)6)22-18(20)12-9-11-17(19)21-15(8-2)13(3)4/h13-1
InchiKey:	QYVYFZNBYOGCKA-UHFFFAOYSA-N
Formula:	C18H34O4
SMILES:	CCCC(OC(=O)CCCC(=O)OC(CC)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	-4.82		Crippen Method
logp	4.502		Crippen Method
mcvol	279.360	ml/mol	McGowan Method
pc	1255.70	kPa	Joback Method
rinpola	1865.00		NIST Webbook
tb	762.06	K	Joback Method
tc	946.82	K	Joback Method
tf	376.94	K	Joback Method
vc	1.067	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	851.43	J/molxK	762.06	Joback Method
cpg	869.48	J/molxK	792.85	Joback Method
cpg	886.51	J/molxK	823.65	Joback Method
cpg	902.54	J/molxK	854.44	Joback Method
cpg	917.58	J/molxK	885.24	Joback Method
cpg	931.65	J/molxK	916.03	Joback Method
cpg	944.75	J/molxK	946.82	Joback Method
dvisc	0.0024596	Paxs	376.94	Joback Method
dvisc	0.0008051	Paxs	441.13	Joback Method

dvisc	0.0003500	Paxs	505.31	Joback Method
dvisc	0.0001836	Paxs	569.50	Joback Method
dvisc	0.0001097	Paxs	633.69	Joback Method
dvisc	0.0000721	Paxs	697.87	Joback Method
dvisc	0.0000509	Paxs	762.06	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393729&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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