

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

Inchi: InChI=1S/C19H36O4/c1-6-8-9-10-12-16(5)22-18(20)13-11-14-19(21)23-17(7-2)15(3)4/h1-5,7-10,12-16,18-20,22-23,25-26,28-29,31-32H,17,21,24,27,30,33H2,34H3
InchiKey: KGFMQDGAKDRSRQ-UHFFFAOYSA-N
Formula: C19H36O4
SMILES: CCCCCC(C)OC(=O)CCCC(=O)OC(CC)C(C)C
Mol. weight [g/mol]: 328.49

Physical Properties

Property code	Value	Unit	Source
gf	-366.06	kJ/mol	Joback Method
hf	-940.93	kJ/mol	Joback Method
hfus	39.97	kJ/mol	Joback Method
hvap	75.04	kJ/mol	Joback Method
log10ws	-5.48		Crippen Method
logp	5.037		Crippen Method
mvol	293.450	ml/mol	McGowan Method
pc	1168.02	kPa	Joback Method
rinpol	2041.00		NIST Webbook
rinpol	2041.00		NIST Webbook
tb	785.38	K	Joback Method
tc	969.72	K	Joback Method
tf	403.21	K	Joback Method
vc	1.129	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	910.35	J/molxK	785.38	Joback Method
cpg	991.06	J/molxK	939.00	Joback Method
cpg	976.93	J/molxK	908.28	Joback Method
cpg	961.82	J/molxK	877.55	Joback Method
cpg	945.69	J/molxK	846.83	Joback Method
cpg	928.54	J/molxK	816.10	Joback Method
cpg	1004.20	J/molxK	969.72	Joback Method
dvisc	0.0000478	Paxs	785.38	Joback Method

dvisc	0.0000666	Paxs	721.68	Joback Method
dvisc	0.0000989	Paxs	657.99	Joback Method
dvisc	0.0001598	Paxs	594.29	Joback Method
dvisc	0.0002900	Paxs	530.60	Joback Method
dvisc	0.0006190	Paxs	466.90	Joback Method
dvisc	0.0016792	Paxs	403.21	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=U391447&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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