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

Inchi: InChI=1S/C19H36O4/c1-8-10-16(14(2)3)23-18(21)12-9-11-17(20)22-15(4)13-19(5,6)7/h1

InchiKey: MKQAKDBWOGDUOP-UHFFFAOYSA-N

Formula: C19H36O4

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

Mol. weight [g/mol]: 328.49

Physical Properties

Property code	Value	Unit	Source
gf	-363.22	kJ/mol	Joback Method
hf	-949.68	kJ/mol	Joback Method
hfus	32.56	kJ/mol	Joback Method
hvap	73.74	kJ/mol	Joback Method
log10ws	-5.24		Crippen Method
logp	4.893		Crippen Method
mcvol	293.450	ml/mol	McGowan Method
pc	1183.34	kPa	Joback Method
rinpol	2145.00		NIST Webbook
tb	782.15	K	Joback Method
tc	970.65	K	Joback Method
tf	405.63	K	Joback Method
vc	1.119	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	911.64	J/mol×K	782.15	Joback Method
cpg	992.90	J/mol×K	939.23	Joback Method
cpg	978.69	J/mol×K	907.82	Joback Method
cpg	963.49	J/mol×K	876.40	Joback Method
cpg	947.26	J/mol×K	844.98	Joback Method
cpg	929.99	J/mol×K	813.57	Joback Method
cpg	1006.14	J/mol×K	970.65	Joback Method
dvisc	0.0000387	Pa×s	782.15	Joback Method
dvisc	0.0000552	Pa×s	719.40	Joback Method

dvisc	0.0000844	Pa×s	656.64	Joback Method
dvisc	0.0001410	Pa×s	593.89	Joback Method
dvisc	0.0002659	Pa×s	531.14	Joback Method
dvisc	0.0005945	Pa×s	468.38	Joback Method
dvisc	0.0017052	Pa×s	405.63	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377603&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

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