

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

Inchi:	InChI=1S/C20H38O4/c1-8-10-17(15(2)3)24-19(22)12-9-11-18(21)23-14-16(4)13-20(5,6)7
InchiKey:	UGESDFFYQZYVRC-UHFFFAOYSA-N
Formula:	C20H38O4
SMILES:	CCCC(OC(=O)CCCC(=O)OCC(C)CC(C)(C)C)C(C)C
Mol. weight [g/mol]:	342.51

Physical Properties

Property code	Value	Unit	Source
gf	-354.80	kJ/mol	Joback Method
hf	-970.32	kJ/mol	Joback Method
hfus	35.15	kJ/mol	Joback Method
hvap	75.97	kJ/mol	Joback Method
log10ws	-5.31		Crippen Method
logp	5.140		Crippen Method
mcvol	307.540	ml/mol	McGowan Method
pc	1108.89	kPa	Joback Method
rinpola	2121.00		NIST Webbook
tb	805.03	K	Joback Method
tc	994.59	K	Joback Method
tf	416.90	K	Joback Method
vc	1.175	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	971.63	J/molxK	805.03	Joback Method
cpg	1053.76	J/molxK	963.00	Joback Method
cpg	1039.44	J/molxK	931.40	Joback Method
cpg	1024.11	J/molxK	899.81	Joback Method
cpg	1007.71	J/molxK	868.22	Joback Method
cpg	990.23	J/molxK	836.62	Joback Method
cpg	1067.08	J/molxK	994.59	Joback Method
dvisc	0.0000331	Paxs	805.03	Joback Method
dvisc	0.0000473	Paxs	740.34	Joback Method

dvisc	0.0000723	Paxs	675.65	Joback Method
dvisc	0.0001209	Paxs	610.96	Joback Method
dvisc	0.0002286	Paxs	546.28	Joback Method
dvisc	0.0005125	Paxs	481.59	Joback Method
dvisc	0.0014766	Paxs	416.90	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377225&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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