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

Inchi: InChI=1S/C20H38O4/c1-7-9-11-17(8-2)14-23-18(21)12-10-13-19(22)24-20(15(3)4)16(5)6

InchiKey: VOQIUEARBRVCPB-UHFFFAOYSA-N

Formula: C20H38O4

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

Mol. weight [g/mol]: 342.51

Physical Properties

Property code	Value	Unit	Source
gf	-360.08	kJ/mol	Joback Method
hf	-966.85	kJ/mol	Joback Method
hfus	39.04	kJ/mol	Joback Method
hvap	76.87	kJ/mol	Joback Method
log10ws	-5.31		Crippen Method
logp	5.140		Crippen Method
mcvol	307.540	ml/mol	McGowan Method
pc	1100.81	kPa	Joback Method
rinpol	2105.00		NIST Webbook
rinpol	2105.00		NIST Webbook
tb	807.82	K	Joback Method
tc	995.23	K	Joback Method
tf	399.48	K	Joback Method
vc	1.179	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	971.09	J/mol×K	807.82	Joback Method
cpg	989.72	J/mol×K	839.05	Joback Method
cpg	1007.22	J/mol×K	870.29	Joback Method
cpg	1023.63	J/mol×K	901.52	Joback Method
cpg	1038.95	J/mol×K	932.76	Joback Method
cpg	1053.20	J/mol×K	963.99	Joback Method
cpg	1066.41	J/mol×K	995.23	Joback Method
dvisc	0.0018698	Pa×s	399.48	Joback Method

dvisc	0.0006083	Pa×s	467.54	Joback Method
dvisc	0.0002633	Pa×s	535.59	Joback Method
dvisc	0.0001376	Pa×s	603.65	Joback Method
dvisc	0.0000821	Pa×s	671.71	Joback Method
dvisc	0.0000538	Pa×s	739.76	Joback Method
dvisc	0.0000379	Pa×s	807.82	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393478&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

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