Pentanedioic acid, bis(2-methylpropyl) ester

Other names: Diisobutyl glutarate
Inchi: InChI=1S/C13H24O4/c1-10(2)8-16-12(14)6-5-7-13(15)17-9-11(3)4/h10-11H,5-9H2,1-4H3
InchiKey: UFWRCRCDRAUAAO-UHFFFAOYSA-N
Formula: C13H24O4
SMILES: CC(C)COC(=O)CCCC(=O)OCC(C)C
Mol. weight [g/mol]: 244.33
CAS: 71195-64-7

Physical Properties

Property code	Value	Unit	Source
gf	-414.14	kJ/mol	Joback Method
hf	-811.81	kJ/mol	Joback Method
hfus	27.95	kJ/mol	Joback Method
hvap	62.07	kJ/mol	Joback Method
log10ws	-2.51		Crippen Method
logp	2.555		Crippen Method
mcvol	208.910	ml/mol	McGowan Method
pc	1798.51	kPa	Joback Method
rinpol	1605.00		NIST Webbook
rinpol	1546.00		NIST Webbook
rinpol	1546.00		NIST Webbook
rinpol	1605.00		NIST Webbook
tb	648.54	K	Joback Method
tc	830.39	K	Joback Method
tf	350.59	K	Joback Method
vc	0.799	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	569.26	J/mol×K	648.54	Joback Method
cpg	584.92	J/mol×K	678.85	Joback Method
cpg	599.84	J/mol×K	709.16	Joback Method
cpg	614.03	J/mol×K	739.46	Joback Method

cpg	627.48	J/mol×K	769.77	Joback Method
cpg	640.21	J/mol×K	800.08	Joback Method
cpg	652.22	J/mol×K	830.39	Joback Method
dvisc	0.0025317	Pa×s	350.59	Joback Method
dvisc	0.0011034	Pa×s	400.25	Joback Method
dvisc	0.0005777	Pa×s	449.91	Joback Method
dvisc	0.0003440	Pa×s	499.56	Joback Method
dvisc	0.0002249	Pa×s	549.22	Joback Method
dvisc	0.0001578	Pa×s	598.88	Joback Method
dvisc	0.0001169	Pa×s	648.54	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C71195647&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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