Butanedioic acid, diheptyl ester

Other names: diheptyl succinate
Inchi: InChI=1S/C18H34O4/c1-3-5-7-9-11-15-21-17(19)13-14-18(20)22-16-12-10-8-6-4-2/h3-16
InchiKey: PBZAGXRVDLNBCJ-UHFFFAOYSA-N
Formula: C18H34O4
SMILES: CCCCCCCOC(=O)CCC(=O)OCCCCCCC
Mol. weight [g/mol]: 314.46
CAS: 15872-89-6

Physical Properties

Property code	Value	Unit	Source
gf	-367.16	kJ/mol	Joback Method
hf	-904.45	kJ/mol	Joback Method
hfus	47.95	kJ/mol	Joback Method
hvap	73.97	kJ/mol	Joback Method
log10ws	-5.08		Crippen Method
logp	4.794		Crippen Method
mcvol	279.360	ml/mol	McGowan Method
pc	1227.70	kPa	Joback Method
rinpol	2124.00		NIST Webbook
rinpol	2124.00		NIST Webbook
tb	763.82	K	Joback Method
tc	942.53	K	Joback Method
tf	436.94	K	Joback Method
vc	1.091	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	849.49	J/mol×K	763.82	Joback Method
cpg	927.49	J/mol×K	912.75	Joback Method
cpg	913.68	J/mol×K	882.96	Joback Method
cpg	898.98	J/mol×K	853.18	Joback Method
cpg	883.40	J/mol×K	823.39	Joback Method
cpg	866.90	J/mol×K	793.61	Joback Method

cpg	940.44	J/mol×K	942.53	Joback Method
dvisc	0.0000707	Pa×s	763.82	Joback Method
dvisc	0.0000931	Pa×s	709.34	Joback Method
dvisc	0.0001284	Pa×s	654.86	Joback Method
dvisc	0.0001878	Pa×s	600.38	Joback Method
dvisc	0.0002962	Pa×s	545.90	Joback Method
dvisc	0.0005169	Pa×s	491.42	Joback Method
dvisc	0.0010365	Pa×s	436.94	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=C15872896&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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