Butanedioic acid, dihexyl ester

Other names: Dihexyl succinate
Inchi: InChI=1S/C16H30O4/c1-3-5-7-9-13-19-15(17)11-12-16(18)20-14-10-8-6-4-2/h3-14H2,1-2
InchiKey: XEYHWMQDXTVNJW-UHFFFAOYSA-N
Formula: C16H30O4
SMILES: CCCCCCOC(=O)CCC(=O)OCCCCCC
Mol. weight [g/mol]: 286.41
CAS: 15805-75-1

Physical Properties

Property code	Value	Unit	Source
gf	-384.00	kJ/mol	Joback Method
hf	-863.17	kJ/mol	Joback Method
hfus	42.77	kJ/mol	Joback Method
hvap	69.52	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	4.014		Crippen Method
mcvol	251.180	ml/mol	McGowan Method
pc	1411.18	kPa	Joback Method
rinpol	1941.00		NIST Webbook
rinpol	1910.00		NIST Webbook
tb	718.06	K	Joback Method
tc	894.33	K	Joback Method
tf	414.40	K	Joback Method
vc	0.980	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	733.60	J/mol×K	718.06	Joback Method
cpg	750.17	J/mol×K	747.44	Joback Method
cpg	765.92	J/mol×K	776.82	Joback Method
cpg	780.87	J/mol×K	806.19	Joback Method
cpg	795.02	J/mol×K	835.57	Joback Method
cpg	808.37	J/mol×K	864.95	Joback Method

cpg	820.95	J/mol×K	894.33	Joback Method
dvisc	0.0012551	Pa×s	414.40	Joback Method
dvisc	0.0006418	Pa×s	465.01	Joback Method
dvisc	0.0003744	Pa×s	515.62	Joback Method
dvisc	0.0002405	Pa×s	566.23	Joback Method
dvisc	0.0001661	Pa×s	616.84	Joback Method
dvisc	0.0001214	Pa×s	667.45	Joback Method
dvisc	0.0000927	Pa×s	718.06	Joback Method

Sources

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=C15805751&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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