Hexanedioic acid, bis(2-butoxyethyl) ester

Other names:	Hexanedioic acid, bis(2-butoxyethyl) ester
	Adipic acid, bis(ethylene glycol monobutyl ether) ester
	Adipic acid, bis(2-butoxyethyl) ester
	Adipic acid, bis(2-butyoxyethyl) ester
	Adipic acid, dibutoxyethyl ester
	Adipol BCA
	Bis(ethylene glycol monobutyl ether) adipate
	Bis(2-butoxyethyl) adipate
	Butyl "Cellosolve" Adipate (BCA)
	Di(2-butoxyethyl) adipate
	Dibutyl Cellosolve Adipate
	Staflex DBEA
	Butyl "cellosolve" adipate
	Adipic acid, di(2-butoxyethyl) ester
	Hexanedioic acid, 1,6-bis(2-butoxyethyl) ester
	NSC 4813
Inchi:	InChI=1S/C18H34O6/c1-3-5-11-21-13-15-23-17(19)9-7-8-10-18(20)24-16-14-22-12-6-4-2
InchiKey:	IHTSDBYPAZEUOP-UHFFFAOYSA-N
Formula:	C18H34O6
SMILES:	CCCCOCCOC(=O)CCCCC(=O)OCCOCCCC
Mol. weight [g/mol]:	346.46

Physical Properties

Property code	Value	Unit	Source
af	1.0522		Cheméo Relay (1.0)
gf	-577.16	kJ/mol	Joback Method
hf	-1278.18	kJ/mol	Cheméo Relay (1.0)
hfus	50.33	kJ/mol	Joback Method
hvap	98.46	kJ/mol	Cheméo Relay (1.0)
ie	9.39	eV	Cheméo Relay (1.0)
log10ws	-3.01		Cheméo Relay (1.0)
logp	3.267		Crippen Method
mcvol	291.100	ml/mol	McGowan Method
pc	1198.96	kPa	Joback Method
tb	621.36	K	Cheméo Relay (1.0)
tc	778.18	K	Cheméo Relay (1.0)
tf	235.06	K	Cheméo Relay (1.0)

vc	1.118	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	911.35	J/mol×K	808.66	Joback Method
cpg	928.34	J/mol×K	839.33	Joback Method
cpg	944.28	J/mol×K	869.99	Joback Method
cpg	959.16	J/mol×K	900.66	Joback Method
cpg	972.97	J/mol×K	931.32	Joback Method
cpg	985.71	J/mol×K	961.99	Joback Method
cpg	997.37	J/mol×K	992.65	Joback Method
dvisc	0.0004909	Pa×s	481.40	Joback Method
dvisc	0.0002611	Pa×s	535.94	Joback Method
dvisc	0.0001561	Pa×s	590.49	Joback Method
dvisc	0.0001018	Pa×s	645.03	Joback Method
dvisc	0.0000709	Pa×s	699.57	Joback Method
dvisc	0.0000521	Pa×s	754.12	Joback Method
dvisc	0.0000399	Pa×s	808.66	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C141184&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

af: Acentric Factor

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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume