Nonanedioic acid, dibutyl ester

Other names:	Azelaic acid, dibutyl ester
	Dibutyl azelate
	Dibutyl nonanedioate
	1,9-Di-n-butyl nonanedioate
	Di-n-butyl azelate
	Dibutyl nonadioate
Inchi:	InChI=1S/C17H32O4/c1-3-5-14-20-16(18)12-10-8-7-9-11-13-17(19)21-15-6-4-2/h3-15H2
InchiKey:	RISLXYINQFKFRL-UHFFFAOYSA-N
Formula:	C17H32O4
SMILES:	CCCCOC(=O)CCCCCCCC(=O)OCCCC
Mol. weight [g/mol]:	300.43
CAS:	2917-73-9

Physical Properties

Property code	Value	Unit	Source
gf	-375.58	kJ/mol	Joback Method
hf	-883.81	kJ/mol	Joback Method
hfus	45.36	kJ/mol	Joback Method
hvap	71.75	kJ/mol	Joback Method
log10ws	-4.66		Crippen Method
logp	4.404		Crippen Method
mcvol	265.270	ml/mol	McGowan Method
pc	1314.65	kPa	Joback Method
rinpol	2029.00		NIST Webbook
tb	740.94	K	Joback Method
tc	918.14	K	Joback Method
tf	425.67	K	Joback Method
vc	1.036	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	880.23	J/mol×K	918.14	Joback Method
cpg	867.46	J/mol×K	888.60	Joback Method

cpg	853.86	J/mol×K	859.07	Joback Method
cpg	839.43	J/mol×K	829.54	Joback Method
cpg	824.15	J/mol×K	800.01	Joback Method
cpg	808.03	J/mol×K	770.47	Joback Method
cpg	791.03	J/mol×K	740.94	Joback Method
dvisc	0.0011435	Pa×s	425.67	Joback Method
dvisc	0.0000811	Pa×s	740.94	Joback Method
dvisc	0.0001065	Pa×s	688.39	Joback Method
dvisc	0.0001463	Pa×s	635.85	Joback Method
dvisc	0.0002129	Pa×s	583.31	Joback Method
dvisc	0.0003337	Pa×s	530.76	Joback Method
dvisc	0.0005773	Pa×s	478.21	Joback Method
hvapt	88.40	kJ/mol	381.50	NIST Webbook

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=C2917739&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
hvapt: Enthalpy of vaporization at a given temperature
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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