ENT-337

Other names:	Malic acid, dibutyl ester, (.+/-.)-
	Butanedioic acid, hydroxy-, dibutyl ester, (.+/-.)-
	Dibutyl malate
	DL-Malic acid, di-n-butyl ester
	NSC 6194
	dibutyl (±)-malate
Inchi:	InChI=1S/C12H22O5/c1-3-5-7-16-11(14)9-10(13)12(15)17-8-6-4-2/h10,13H,3-9H2,1-2H3
InchiKey:	PDSCSYLDRHAHOX-UHFFFAOYSA-N
Formula:	C12H22O5
SMILES:	CCCCOC(=O)CC(O)C(=O)OCCCC
Mol. weight [g/mol]:	246.30
CAS:	6280-99-5

Physical Properties

Property code	Value	Unit	Source
gf	-556.94	kJ/mol	Joback Method
hf	-938.12	kJ/mol	Joback Method
hfus	32.97	kJ/mol	Joback Method
hvap	76.91	kJ/mol	Joback Method
log10ws	-1.95		Crippen Method
logp	1.424		Crippen Method
mcvol	200.690	ml/mol	McGowan Method
pc	2108.07	kPa	Joback Method
tb	718.28	K	Joback Method
tc	895.67	K	Joback Method
tf	415.14	K	Joback Method
vc	0.768	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	577.43	J/mol×K	718.28	Joback Method
cpg	590.18	J/mol×K	747.85	Joback Method
cpg	602.29	J/mol×K	777.41	Joback Method

cpg	613.74	J/mol×K	806.98	Joback Method
cpg	624.55	J/mol×K	836.54	Joback Method
cpg	634.71	J/mol×K	866.11	Joback Method
cpg	644.22	J/mol×K	895.67	Joback Method
dvisc	0.0016760	Pa×s	415.14	Joback Method
dvisc	0.0005994	Pa×s	465.66	Joback Method
dvisc	0.0002622	Pa×s	516.19	Joback Method
dvisc	0.0001329	Pa×s	566.71	Joback Method
dvisc	0.0000753	Pa×s	617.23	Joback Method
dvisc	0.0000465	Pa×s	667.76	Joback Method
dvisc	0.0000307	Pa×s	718.28	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=C6280995&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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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