Diethylmalonic acid, butyl 2-methylpentyl ester

Inchi: InChI=1S/C17H32O4/c1-6-10-12-20-15(18)17(8-3,9-4)16(19)21-13-14(5)11-7-2/h14H,6-1

InchiKey: GNMOAVVJELTEJH-UHFFFAOYSA-N

Formula: C17H32O4

SMILES: CCCCOC(=O)C(CC)(CC)C(=O)OCC(C)CCC

Mol. weight [g/mol]: 300.43

Physical Properties

Property code	Value	Unit	Source
gf	-375.18	kJ/mol	Joback Method
hf	-897.84	kJ/mol	Joback Method
hfus	34.42	kJ/mol	Joback Method
hvap	70.06	kJ/mol	Joback Method
log10ws	-4.18		Crippen Method
logp	4.115		Crippen Method
mcvol	265.270	ml/mol	McGowan Method
pc	1340.78	kPa	Joback Method
rinpol	1684.00		NIST Webbook
tb	737.27	K	Joback Method
tc	921.13	K	Joback Method
tf	413.09	K	Joback Method
vc	1.018	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	793.34	J/mol×K	737.27	Joback Method
cpg	810.75	J/mol×K	767.91	Joback Method
cpg	827.21	J/mol×K	798.56	Joback Method
cpg	842.74	J/mol×K	829.20	Joback Method
cpg	857.37	J/mol×K	859.84	Joback Method
cpg	871.12	J/mol×K	890.49	Joback Method
cpg	884.02	J/mol×K	921.13	Joback Method
dvisc	0.0013901	Pa×s	413.09	Joback Method
dvisc	0.0006127	Pa×s	467.12	Joback Method

dvisc	0.0003200	Pa×s	521.15	Joback Method
dvisc	0.0001889	Pa×s	575.18	Joback Method
dvisc	0.0001220	Pa×s	629.21	Joback Method
dvisc	0.0000845	Pa×s	683.24	Joback Method
dvisc	0.0000617	Pa×s	737.27	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=U369757&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

Latest version available from:
https://www.chemeo.com/cid/16-861-8/Diethylmalonic-acid-butyl-2-methylpentyl-ester.pdf
Generated by Cheméo on 2024-10-12 03:48:04.862193534 +0000 UTC m=+3285747.499162786.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.