Diethylmalonic acid, butyl 4-methylpent-2-yl ester

Inchi: InChI=1S/C17H32O4/c1-7-10-11-20-15(18)17(8-2,9-3)16(19)21-14(6)12-13(4)5/h13-14H

InchiKey: NXHOLAOHAXLAJF-UHFFFAOYSA-N

Formula: C17H32O4

SMILES: CCCCOC(=O)C(CC)(CC)C(=O)OC(C)CC(C)C

Mol. weight [g/mol]: 300.43

Physical Properties

Property code	Value	Unit	Source
gf	-377.62	kJ/mol	Joback Method
hf	-903.12	kJ/mol	Joback Method
hfus	30.90	kJ/mol	Joback Method
hvap	69.68	kJ/mol	Joback Method
log10ws	-4.29		Crippen Method
logp	4.114		Crippen Method
mcvol	265.270	ml/mol	McGowan Method
pc	1348.67	kPa	Joback Method
rinpol	1645.00		NIST Webbook
rinpol	1645.00		NIST Webbook
tb	736.83	K	Joback Method
tc	922.80	K	Joback Method
tf	398.09	K	Joback Method
vc	1.012	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	793.82	J/mol×K	736.83	Joback Method
cpg	872.39	J/mol×K	891.80	Joback Method
cpg	858.54	J/mol×K	860.81	Joback Method
cpg	843.79	J/mol×K	829.81	Joback Method
cpg	828.10	J/mol×K	798.82	Joback Method
cpg	811.45	J/mol×K	767.82	Joback Method
cpg	885.36	J/mol×K	922.80	Joback Method
dvisc	0.0000570	Pa×s	736.83	Joback Method

dvisc	0.0000795	Pa×s	680.37	Joback Method
dvisc	0.0001179	Pa×s	623.92	Joback Method
dvisc	0.0001892	Pa×s	567.46	Joback Method
dvisc	0.0003369	Pa×s	511.00	Joback Method
dvisc	0.0006925	Pa×s	454.55	Joback Method
dvisc	0.0017460	Pa×s	398.09	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370496&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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