Diethylmalonic acid, butyl 2,4,4-trimethylpentyl ester

Inchi: InChI=1S/C19H36O4/c1-8-11-12-22-16(20)19(9-2,10-3)17(21)23-14-15(4)13-18(5,6)7/h1

InchiKey: YXYPVKHNYAXUIS-UHFFFAOYSA-N

Formula: C19H36O4

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

Mol. weight [g/mol]: 328.49

Physical Properties

Property code	Value	Unit	Source
gf	-355.50	kJ/mol	Joback Method
hf	-947.87	kJ/mol	Joback Method
hfus	32.19	kJ/mol	Joback Method
hvap	73.22	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	4.752		Crippen Method
mcvol	293.450	ml/mol	McGowan Method
pc	1185.79	kPa	Joback Method
rinpol	1829.00		NIST Webbook
tb	779.80	K	Joback Method
tc	969.61	K	Joback Method
tf	438.05	K	Joback Method
vc	1.119	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	912.00	J/mol×K	779.80	Joback Method
cpg	930.22	J/mol×K	811.44	Joback Method
cpg	947.36	J/mol×K	843.07	Joback Method
cpg	963.48	J/mol×K	874.71	Joback Method
cpg	978.62	J/mol×K	906.34	Joback Method
cpg	992.81	J/mol×K	937.98	Joback Method
cpg	1006.10	J/mol×K	969.61	Joback Method
dvisc	0.0010640	Pa×s	438.05	Joback Method
dvisc	0.0004408	Pa×s	495.01	Joback Method

dvisc	0.0002190	Pa×s	551.97	Joback Method
dvisc	0.0001240	Pa×s	608.92	Joback Method
dvisc	0.0000774	Pa×s	665.88	Joback Method
dvisc	0.0000521	Pa×s	722.84	Joback Method
dvisc	0.0000371	Pa×s	779.80	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369476&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