Diethylmalonic acid, isobutyl 3-methylbenzyl ester

Inchi: InChI=1S/C19H28O4/c1-6-19(7-2,17(20)22-12-14(3)4)18(21)23-13-16-10-8-9-15(5)11-16

InchiKey: HUVUGUDXCOOVMI-UHFFFAOYSA-N

Formula: C19H28O4

SMILES: CCC(CC)(C(=O)OCc1cccc(C)c1)C(=O)OCC(C)C

Mol. weight [g/mol]: 320.42

Physical Properties

Property code	Value	Unit	Source
gf	-255.56	kJ/mol	Joback Method
hf	-714.06	kJ/mol	Joback Method
hfus	33.25	kJ/mol	Joback Method
hvap	77.45	kJ/mol	Joback Method
log10ws	-4.67		Crippen Method
logp	4.044		Crippen Method
mcvol	269.690	ml/mol	McGowan Method
pc	1471.36	kPa	Joback Method
rinpol	2024.00		NIST Webbook
tb	814.69	K	Joback Method
tc	1022.76	K	Joback Method
tf	474.57	K	Joback Method
vc	1.022	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	820.88	J/mol×K	814.69	Joback Method
cpg	891.18	J/mol×K	988.09	Joback Method
cpg	879.29	J/mol×K	953.41	Joback Method
cpg	866.36	J/mol×K	918.73	Joback Method
cpg	852.34	J/mol×K	884.05	Joback Method
cpg	837.19	J/mol×K	849.37	Joback Method
cpg	902.07	J/mol×K	1022.76	Joback Method
dvisc	0.0000461	Pa×s	814.69	Joback Method
dvisc	0.0000613	Pa×s	758.00	Joback Method

dvisc	0.0000852	Pa×s	701.32	Joback Method
dvisc	0.0001257	Pa×s	644.63	Joback Method
dvisc	0.0001997	Pa×s	587.94	Joback Method
dvisc	0.0003503	Pa×s	531.26	Joback Method
dvisc	0.0007029	Pa×s	474.57	Joback Method

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=U369305&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
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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