Diethylmalonic acid, ethyl 3-methylbenzyl ester

Inchi: InChI=1S/C17H24O4/c1-5-17(6-2,15(18)20-7-3)16(19)21-12-14-10-8-9-13(4)11-14/h8-11

InchiKey: PFTLVKPNEYWMPF-UHFFFAOYSA-N

Formula: C17H24O4

SMILES: CCOC(=O)C(CC)(CC)C(=O)OCc1cccc(C)c1

Mol. weight [g/mol]: 292.37

Physical Properties

Property code	Value	Unit	Source
gf	-269.96	kJ/mol	Joback Method
hf	-667.50	kJ/mol	Joback Method
hfus	31.60	kJ/mol	Joback Method
hvap	73.39	kJ/mol	Joback Method
log10ws	-4.08		Crippen Method
logp	3.408		Crippen Method
mcvol	241.510	ml/mol	McGowan Method
pc	1703.31	kPa	Joback Method
rinpol	1891.00		NIST Webbook
rinpol	1891.00		NIST Webbook
tb	769.37	K	Joback Method
tc	977.67	K	Joback Method
tf	467.03	K	Joback Method
vc	0.916	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	706.20	J/mol×K	769.37	Joback Method
cpg	721.92	J/mol×K	804.09	Joback Method
cpg	736.56	J/mol×K	838.80	Joback Method
cpg	750.15	J/mol×K	873.52	Joback Method
cpg	762.72	J/mol×K	908.23	Joback Method
cpg	774.31	J/mol×K	942.95	Joback Method
cpg	784.95	J/mol×K	977.67	Joback Method
dvisc	0.0007474	Pa×s	467.03	Joback Method

dvisc	0.0004108	Pa×s	517.42	Joback Method
dvisc	0.0002511	Pa×s	567.81	Joback Method
dvisc	0.0001663	Pa×s	618.20	Joback Method
dvisc	0.0001172	Pa×s	668.59	Joback Method
dvisc	0.0000867	Pa×s	718.98	Joback Method
dvisc	0.0000668	Pa×s	769.37	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=U369303&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