Diethylmalonic acid, isobutyl 3-methoxyphenyl ester

Inchi: InChI=1S/C18H26O5/c1-6-18(7-2,16(19)22-12-13(3)4)17(20)23-15-10-8-9-14(11-15)21-5

InchiKey: IWYLHMKCPCZBRC-UHFFFAOYSA-N

Formula: C18H26O5

SMILES: CCC(CC)(C(=O)OCC(C)C)C(=O)Oc1cccc(OC)c1

Mol. weight [g/mol]: 322.40

Physical Properties

Property code	Value	Unit	Source
gf	-368.98	kJ/mol	Joback Method
hf	-825.64	kJ/mol	Joback Method
hfus	31.85	kJ/mol	Joback Method
hvap	77.64	kJ/mol	Joback Method
log10ws	-4.05		Crippen Method
logp	3.606		Crippen Method
mcvol	261.470	ml/mol	McGowan Method
pc	1564.75	kPa	Joback Method
rinpol	2113.00		NIST Webbook
tb	814.23	K	Joback Method
tc	1022.96	K	Joback Method
tf	485.53	K	Joback Method
vc	0.985	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	791.91	J/mol×K	814.23	Joback Method
cpg	858.44	J/mol×K	988.17	Joback Method
cpg	847.41	J/mol×K	953.38	Joback Method
cpg	835.26	J/mol×K	918.59	Joback Method
cpg	821.97	J/mol×K	883.81	Joback Method
cpg	807.53	J/mol×K	849.02	Joback Method
cpg	868.39	J/mol×K	1022.96	Joback Method
dvisc	0.0000399	Pa×s	814.23	Joback Method
dvisc	0.0000526	Pa×s	759.45	Joback Method

dvisc	0.0000725	Pa×s	704.66	Joback Method
dvisc	0.0001053	Pa×s	649.88	Joback Method
dvisc	0.0001640	Pa×s	595.10	Joback Method
dvisc	0.0002792	Pa×s	540.31	Joback Method
dvisc	0.0005362	Pa×s	485.53	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=U370870&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