Diethylmalonic acid, butyl 3-methoxyphenyl ester

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

InchiKey: IAGDDNYENWZNOX-UHFFFAOYSA-N

Formula: C18H26O5

SMILES: CCCCOC(=O)C(CC)(CC)C(=O)Oc1cccc(OC)c1

Mol. weight [g/mol]: 322.40

Physical Properties

Property code	Value	Unit	Source
gf	-366.54	kJ/mol	Joback Method
hf	-820.36	kJ/mol	Joback Method
hfus	35.38	kJ/mol	Joback Method
hvap	78.03	kJ/mol	Joback Method
log10ws	-4.29		Crippen Method
logp	3.750		Crippen Method
mcvol	261.470	ml/mol	McGowan Method
pc	1554.90	kPa	Joback Method
rinpol	2146.00		NIST Webbook
rinpol	2146.00		NIST Webbook
tb	814.67	K	Joback Method
tc	1020.88	K	Joback Method
tf	500.53	K	Joback Method
vc	0.991	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	791.37	J/mol×K	814.67	Joback Method
cpg	806.81	J/mol×K	849.04	Joback Method
cpg	821.11	J/mol×K	883.41	Joback Method
cpg	834.29	J/mol×K	917.77	Joback Method
cpg	846.37	J/mol×K	952.14	Joback Method
cpg	857.37	J/mol×K	986.51	Joback Method
cpg	867.33	J/mol×K	1020.88	Joback Method
dvisc	0.0004688	Pa×s	500.53	Joback Method

dvisc	0.0002614	Pa×s	552.89	Joback Method
dvisc	0.0001613	Pa×s	605.24	Joback Method
dvisc	0.0001075	Pa×s	657.60	Joback Method
dvisc	0.0000760	Pa×s	709.96	Joback Method
dvisc	0.0000564	Pa×s	762.31	Joback Method
dvisc	0.0000435	Pa×s	814.67	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=U370871&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