Diethylmalonic acid, butyl 2,3-dimethylphenyl ester

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

InchiKey: VPYRUNVYZZHYDN-UHFFFAOYSA-N

Formula: C19H28O4

SMILES: CCCCOC(=O)C(CC)(CC)C(=O)Oc1cccc(C)c1C

Mol. weight [g/mol]: 320.42

Physical Properties

Property code	Value	Unit	Source
gf	-262.75	kJ/mol	Joback Method
hf	-720.25	kJ/mol	Joback Method
hfus	36.39	kJ/mol	Joback Method
hvap	78.50	kJ/mol	Joback Method
log10ws	-5.12		Crippen Method
logp	4.359		Crippen Method
mcvol	269.690	ml/mol	McGowan Method
pc	1445.73	kPa	Joback Method
rinpol	2113.00		NIST Webbook
tb	820.11	K	Joback Method
tc	1026.51	K	Joback Method
tf	502.09	K	Joback Method
vc	1.028	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	819.64	J/mol×K	820.11	Joback Method
cpg	835.67	J/mol×K	854.51	Joback Method
cpg	850.58	J/mol×K	888.91	Joback Method
cpg	864.40	J/mol×K	923.31	Joback Method
cpg	877.16	J/mol×K	957.71	Joback Method
cpg	888.90	J/mol×K	992.11	Joback Method
cpg	899.65	J/mol×K	1026.51	Joback Method
dvisc	0.0005170	Pa×s	502.09	Joback Method
dvisc	0.0002918	Pa×s	555.09	Joback Method

dvisc	0.0001820	Pa×s	608.10	Joback Method
dvisc	0.0001224	Pa×s	661.10	Joback Method
dvisc	0.0000873	Pa×s	714.10	Joback Method
dvisc	0.0000653	Pa×s	767.11	Joback Method
dvisc	0.0000507	Pa×s	820.11	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370565&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