Diethylmalonic acid, 2,3-dimethylphenyl isobutyl ester

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

InchiKey: FRIUIKLUHCTQSV-UHFFFAOYSA-N

Formula: C19H28O4

SMILES: CCC(CC)(C(=O)OCC(C)C)C(=O)Oc1cccc(C)c1C

Mol. weight [g/mol]: 320.42

Physical Properties

Property code	Value	Unit	Source
gf	-265.19	kJ/mol	Joback Method
hf	-725.53	kJ/mol	Joback Method
hfus	32.87	kJ/mol	Joback Method
hvap	78.12	kJ/mol	Joback Method
log10ws	-4.88		Crippen Method
logp	4.214		Crippen Method
mcvol	269.690	ml/mol	McGowan Method
pc	1454.57	kPa	Joback Method
rinpol	2074.00		NIST Webbook
tb	819.67	K	Joback Method
tc	1028.54	K	Joback Method
tf	487.09	K	Joback Method
vc	1.022	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	820.17	J/mol×K	819.67	Joback Method
cpg	836.38	J/mol×K	854.48	Joback Method
cpg	851.44	J/mol×K	889.29	Joback Method
cpg	865.36	J/mol×K	924.11	Joback Method
cpg	878.20	J/mol×K	958.92	Joback Method
cpg	889.98	J/mol×K	993.73	Joback Method
cpg	900.74	J/mol×K	1028.54	Joback Method
dvisc	0.0005877	Pa×s	487.09	Joback Method
dvisc	0.0003103	Pa×s	542.52	Joback Method

dvisc	0.0001844	Pa×s	597.95	Joback Method
dvisc	0.0001197	Pa×s	653.38	Joback Method
dvisc	0.0000831	Pa×s	708.81	Joback Method
dvisc	0.0000609	Pa×s	764.24	Joback Method
dvisc	0.0000465	Pa×s	819.67	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370564&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