Diethylmalonic acid, butyl 2-isopropylphenyl ester

Inchi: InChI=1S/C20H30O4/c1-6-9-14-23-18(21)20(7-2,8-3)19(22)24-17-13-11-10-12-16(17)15(
InchiKey: CEGNENQCZBWOPH-UHFFFAOYSA-N
Formula: C20H30O4
SMILES: CCCCOC(=O)C(CC)(CC)C(=O)Oc1ccccc1C(C)C
Mol. weight [g/mol]: 334.45

Physical Properties

Property code	Value	Unit	Source
gf	-247.14	kJ/mol	Joback Method
hf	-734.70	kJ/mol	Joback Method
hfus	35.84	kJ/mol	Joback Method
hvap	79.68	kJ/mol	Joback Method
log10ws	-5.36		Crippen Method
logp	4.865		Crippen Method
mcvol	283.780	ml/mol	McGowan Method
pc	1368.70	kPa	Joback Method
rinpol	2033.00		NIST Webbook
tb	837.57	K	Joback Method
tc	1044.90	K	Joback Method
tf	485.84	K	Joback Method
vc	1.079	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	879.27	J/mol×K	837.57	Joback Method
cpg	895.72	J/mol×K	872.13	Joback Method
cpg	910.98	J/mol×K	906.68	Joback Method
cpg	925.11	J/mol×K	941.24	Joback Method
cpg	938.13	J/mol×K	975.79	Joback Method
cpg	950.10	J/mol×K	1010.35	Joback Method
cpg	961.05	J/mol×K	1044.90	Joback Method
dvisc	0.0006273	Pa×s	485.84	Joback Method
dvisc	0.0003093	Pa×s	544.46	Joback Method

dvisc	0.0001750	Pa×s	603.08	Joback Method
dvisc	0.0001095	Pa×s	661.70	Joback Method
dvisc	0.0000740	Pa×s	720.33	Joback Method
dvisc	0.0000530	Pa×s	778.95	Joback Method
dvisc	0.0000398	Pa×s	837.57	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=U369968&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