Diethylmalonic acid, butyl 1-phenylpropyl ester

Inchi: InChI=1S/C20H30O4/c1-5-9-15-23-18(21)20(7-3,8-4)19(22)24-17(6-2)16-13-11-10-12-14

InchiKey: HLHGTGYNALSKDU-UHFFFAOYSA-N

Formula: C20H30O4

SMILES: CCCCOC(=O)C(CC)(CC)C(=O)OC(CC)c1ccccc1

Mol. weight [g/mol]: 334.45

Physical Properties

Property code	Value	Unit	Source
gf	-237.51	kJ/mol	Joback Method
hf	-723.23	kJ/mol	Joback Method
hfus	36.23	kJ/mol	Joback Method
hvap	79.02	kJ/mol	Joback Method
log10ws	-5.24		Crippen Method
logp	4.831		Crippen Method
mcvol	283.780	ml/mol	McGowan Method
pc	1384.02	kPa	Joback Method
rinpol	2041.00		NIST Webbook
tb	832.59	K	Joback Method
tc	1039.11	K	Joback Method
tf	473.32	K	Joback Method
vc	1.079	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	879.92	J/mol×K	832.59	Joback Method
cpg	951.25	J/mol×K	1004.69	Joback Method
cpg	939.17	J/mol×K	970.27	Joback Method
cpg	926.04	J/mol×K	935.85	Joback Method
cpg	911.82	J/mol×K	901.43	Joback Method
cpg	896.46	J/mol×K	867.01	Joback Method
cpg	962.34	J/mol×K	1039.11	Joback Method
dvisc	0.0000394	Pa×s	832.59	Joback Method
dvisc	0.0000533	Pa×s	772.71	Joback Method

dvisc	0.0000758	Pa×s	712.83	Joback Method
dvisc	0.0001150	Pa×s	652.95	Joback Method
dvisc	0.0001899	Pa×s	593.08	Joback Method
dvisc	0.0003508	Pa×s	533.20	Joback Method
dvisc	0.0007571	Pa×s	473.32	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370191&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

Latest version available from:
https://www.chemeo.com/cid/33-247-1/Diethylmalonic-acid-butyl-1-phenylpropyl-ester.pdf
Generated by Cheméo on 2024-04-26 15:30:02.436412491 +0000 UTC m=+16434651.356989807.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.