Dimethylmalonic acid, heptyl 2-isopropoxyphenyl ester

Inchi: InChI=1S/C21H32O5/c1-6-7-8-9-12-15-24-19(22)21(4,5)20(23)26-18-14-11-10-13-17(18)

InchiKey: TVEYSSIOAMQUAA-UHFFFAOYSA-N

Formula: C21H32O5

SMILES: CCCCCCCOC(=O)C(C)(C)C(=O)Oc1ccccc1OC(C)C

Mol. weight [g/mol]: 364.48

Physical Properties

Property code	Value	Unit	Source
gf	-343.72	kJ/mol	Joback Method
hf	-887.56	kJ/mol	Joback Method
hfus	39.62	kJ/mol	Joback Method
hvap	84.32	kJ/mol	Joback Method
log10ws	-5.66		Crippen Method
logp	4.919		Crippen Method
mcvol	303.740	ml/mol	McGowan Method
pc	1261.06	kPa	Joback Method
rinpol	2266.00		NIST Webbook
tb	882.87	K	Joback Method
tc	1091.16	K	Joback Method
tf	519.34	K	Joback Method
vc	1.153	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	967.85	J/mol×K	882.87	Joback Method
cpg	983.85	J/mol×K	917.58	Joback Method
cpg	998.55	J/mol×K	952.30	Joback Method
cpg	1012.00	J/mol×K	987.01	Joback Method
cpg	1024.23	J/mol×K	1021.73	Joback Method
cpg	1035.26	J/mol×K	1056.44	Joback Method
cpg	1045.14	J/mol×K	1091.16	Joback Method
dvisc	0.0003781	Pa×s	519.34	Joback Method
dvisc	0.0001905	Pa×s	579.93	Joback Method

dvisc	0.0001093	Pa×s	640.52	Joback Method
dvisc	0.0000690	Pa×s	701.10	Joback Method
dvisc	0.0000469	Pa×s	761.69	Joback Method
dvisc	0.0000337	Pa×s	822.28	Joback Method
dvisc	0.0000254	Pa×s	882.87	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=U361855&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

Latest version available from:
https://www.chemeo.com/cid/39-272-7/Dimethylmalonic-acid-heptyl-2-isopropoxyphenyl-ester.pdf
Generated by Cheméo on 2024-04-24 20:36:48.085541978 +0000 UTC m=+16280257.006119299.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.