Diethylmalonic acid, di(5-methoxy-3-methylpentyl) ester

Inchi: InChI=1S/C21H40O6/c1-7-21(8-2,19(22)26-15-11-17(3)9-13-24-5)20(23)27-16-12-18(4)1

InchiKey: SPSYZNSKQBSKDA-UHFFFAOYSA-N

Formula: C21H40O6

SMILES: CCC(CC)(C(=O)OCCC(C)CCOC)C(=O)OCCC(C)CCOC

Mol. weight [g/mol]: 388.54

Physical Properties

Property code	Value	Unit	Source
gf	-553.94	kJ/mol	Joback Method
hf	-1250.12	kJ/mol	Joback Method
hfus	43.64	kJ/mol	Joback Method
hvap	83.40	kJ/mol	Joback Method
log10ws	-3.79		Crippen Method
logp	4.005		Crippen Method
mcvol	333.370	ml/mol	McGowan Method
pc	1013.59	kPa	Joback Method
rinpol	2277.00		NIST Webbook
tb	873.19	K	Joback Method
tc	1069.93	K	Joback Method
tf	487.63	K	Joback Method
vc	1.272	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1095.07	J/mol×K	873.19	Joback Method
cpg	1113.06	J/mol×K	905.98	Joback Method
cpg	1129.72	J/mol×K	938.77	Joback Method
cpg	1145.06	J/mol×K	971.56	Joback Method
cpg	1159.11	J/mol×K	1004.35	Joback Method
cpg	1171.87	J/mol×K	1037.14	Joback Method
cpg	1183.36	J/mol×K	1069.93	Joback Method
dvisc	0.0004285	Pa×s	487.63	Joback Method
dvisc	0.0001820	Pa×s	551.89	Joback Method

dvisc	0.0000925	Pa×s	616.15	Joback Method
dvisc	0.0000534	Pa×s	680.41	Joback Method
dvisc	0.0000339	Pa×s	744.67	Joback Method
dvisc	0.0000231	Pa×s	808.93	Joback Method
dvisc	0.0000167	Pa×s	873.19	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370773&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