Diethylmalonic acid, heptyl 5-methoxy-3-methylpentyl ester

Inchi: InChI=1S/C21H40O5/c1-6-9-10-11-12-15-25-19(22)21(7-2,8-3)20(23)26-17-14-18(4)13-1

InchiKey: UJNURMSCZMKUMR-UHFFFAOYSA-N

Formula: C21H40O5

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

Mol. weight [g/mol]: 372.54

Physical Properties

Property code	Value	Unit	Source
gf	-446.50	kJ/mol	Joback Method
hf	-1112.62	kJ/mol	Joback Method
hfus	45.97	kJ/mol	Joback Method
hvap	81.38	kJ/mol	Joback Method
log10ws	-4.94		Crippen Method
logp	4.912		Crippen Method
mcvol	327.500	ml/mol	McGowan Method
pc	1019.43	kPa	Joback Method
rinpol	2206.00		NIST Webbook
tb	851.21	K	Joback Method
tc	1043.75	K	Joback Method
tf	480.40	K	Joback Method
vc	1.260	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1063.19	J/mol×K	851.21	Joback Method
cpg	1081.54	J/mol×K	883.30	Joback Method
cpg	1098.68	J/mol×K	915.39	Joback Method
cpg	1114.64	J/mol×K	947.48	Joback Method
cpg	1129.44	J/mol×K	979.57	Joback Method
cpg	1143.12	J/mol×K	1011.66	Joback Method
cpg	1155.70	J/mol×K	1043.75	Joback Method
dvisc	0.0005533	Pa×s	480.40	Joback Method
dvisc	0.0002455	Pa×s	542.20	Joback Method

dvisc	0.0001286	Pa×s	604.00	Joback Method
dvisc	0.0000760	Pa×s	665.81	Joback Method
dvisc	0.0000491	Pa×s	727.61	Joback Method
dvisc	0.0000340	Pa×s	789.41	Joback Method
dvisc	0.0000248	Pa×s	851.21	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=U370767&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