Diethylmalonic acid, hexyl octyl ester

Inchi: InChI=1S/C21H40O4/c1-5-9-11-13-14-16-18-25-20(23)21(7-3,8-4)19(22)24-17-15-12-10-
InchiKey: IZZNIXUHIZGHRF-UHFFFAOYSA-N
Formula: C21H40O4
SMILES: CCCCCCCCOC(=O)C(CC)(CC)C(=O)OCCCCCC
Mol. weight [g/mol]: 356.54

Physical Properties

Property code	Value	Unit	Source
gf	-339.06	kJ/mol	Joback Method
hf	-975.12	kJ/mol	Joback Method
hfus	48.31	kJ/mol	Joback Method
hvap	79.36	kJ/mol	Joback Method
log10ws	-6.10		Crippen Method
logp	5.820		Crippen Method
mcvol	321.630	ml/mol	McGowan Method
pc	1025.31	kPa	Joback Method
rinpol	2157.00		NIST Webbook
tb	829.23	K	Joback Method
tc	1017.76	K	Joback Method
tf	473.17	K	Joback Method
vc	1.248	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1031.00	J/mol×K	829.23	Joback Method
cpg	1113.29	J/mol×K	986.33	Joback Method
cpg	1098.90	J/mol×K	954.91	Joback Method
cpg	1083.51	J/mol×K	923.49	Joback Method
cpg	1067.09	J/mol×K	892.07	Joback Method
cpg	1049.60	J/mol×K	860.65	Joback Method
cpg	1126.71	J/mol×K	1017.76	Joback Method
dvisc	0.0000366	Pa×s	829.23	Joback Method
dvisc	0.0000496	Pa×s	769.89	Joback Method

dvisc	0.0000707	Pa×s	710.54	Joback Method
dvisc	0.0001074	Pa×s	651.20	Joback Method
dvisc	0.0001776	Pa×s	591.86	Joback Method
dvisc	0.0003284	Pa×s	532.51	Joback Method
dvisc	0.0007084	Pa×s	473.17	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=U369443&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

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