

Diethylmalonic acid, heptyl phenethyl ester

Inchi:	InChI=1S/C22H34O4/c1-4-7-8-9-13-17-25-20(23)22(5-2,6-3)21(24)26-18-16-19-14-11-10
InchiKey:	VWWXGYNFZDABCL-UHFFFAOYSA-N
Formula:	C22H34O4
SMILES:	CCCCCCCOC(=O)C(CC)(CC)C(=O)OCCc1ccccc1
Mol. weight [g/mol]:	362.50

Physical Properties

Property code	Value	Unit	Source
gf	-218.23	kJ/mol	Joback Method
hf	-759.23	kJ/mol	Joback Method
hfus	44.94	kJ/mol	Joback Method
hvap	83.86	kJ/mol	Joback Method
log10ws	-5.62		Crippen Method
logp	5.092		Crippen Method
mcvol	311.960	ml/mol	McGowan Method
pc	1198.96	kPa	Joback Method
rinsol	2341.00		NIST Webbook
tb	878.79	K	Joback Method
tc	1084.30	K	Joback Method
tf	510.86	K	Joback Method
vc	1.196	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	998.42	J/molxK	878.79	Joback Method
cpg	1015.14	J/molxK	913.04	Joback Method
cpg	1030.66	J/molxK	947.29	Joback Method
cpg	1045.03	J/molxK	981.54	Joback Method
cpg	1058.30	J/molxK	1015.79	Joback Method
cpg	1070.52	J/molxK	1050.05	Joback Method
cpg	1081.75	J/molxK	1084.30	Joback Method
dvisc	0.0005115	Paxs	510.86	Joback Method
dvisc	0.0002510	Paxs	572.18	Joback Method

dvisc	0.0001414	Paxs	633.50	Joback Method
dvisc	0.0000882	Paxs	694.83	Joback Method
dvisc	0.0000593	Paxs	756.15	Joback Method
dvisc	0.0000424	Paxs	817.47	Joback Method
dvisc	0.0000317	Paxs	878.79	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369551&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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