

Diethylmalonic acid, isobutyl undecyl ester

Inchi:	InChI=1S/C22H42O4/c1-6-9-10-11-12-13-14-15-16-17-25-20(23)22(7-2,8-3)21(24)26-18
InchiKey:	QDPQMYCVDRRZAN-UHFFFAOYSA-N
Formula:	C22H42O4
SMILES:	CCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCC(C)C
Mol. weight [g/mol]:	370.57

Physical Properties

Property code	Value	Unit	Source
gf	-333.08	kJ/mol	Joback Method
hf	-1001.04	kJ/mol	Joback Method
hfus	47.37	kJ/mol	Joback Method
hvap	81.19	kJ/mol	Joback Method
log10ws	-6.27		Crippen Method
logp	6.066		Crippen Method
mcvol	335.720	ml/mol	McGowan Method
pc	969.88	kPa	Joback Method
rinsol	2248.00		NIST Webbook
tb	851.67	K	Joback Method
tc	1044.13	K	Joback Method
tf	469.44	K	Joback Method
vc	1.298	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1093.02	J/molxK	851.67	Joback Method
cpg	1176.71	J/molxK	1012.05	Joback Method
cpg	1162.18	J/molxK	979.97	Joback Method
cpg	1146.58	J/molxK	947.90	Joback Method
cpg	1129.88	J/molxK	915.82	Joback Method
cpg	1112.04	J/molxK	883.75	Joback Method
cpg	1190.22	J/molxK	1044.13	Joback Method
dvisc	0.0000287	Paxs	851.67	Joback Method
dvisc	0.0000396	Paxs	787.97	Joback Method

dvisc	0.0000579	Paxs	724.26	Joback Method
dvisc	0.0000910	Paxs	660.56	Joback Method
dvisc	0.0001576	Paxs	596.85	Joback Method
dvisc	0.0003111	Paxs	533.14	Joback Method
dvisc	0.0007385	Paxs	469.44	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=U369429&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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