

Diethylmalonic acid, decyl 4-methylcyclohexyl ester

Inchi:	InChI=1S/C24H44O4/c1-5-8-9-10-11-12-13-14-19-27-22(25)24(6-2,7-3)23(26)28-21-17-1
InchiKey:	AYWQDMRLOQVWCY-UHFFFAOYSA-N
Formula:	C24H44O4
SMILES:	CCCCCCCCCOC(=O)C(CC)(CC)C(=O)OC1CCC(C)CC1
Mol. weight [g/mol]:	396.60

Physical Properties

Property code	Value	Unit	Source
gf	-297.06	kJ/mol	Joback Method
hf	-1003.06	kJ/mol	Joback Method
hfus	48.98	kJ/mol	Joback Method
hvap	86.15	kJ/mol	Joback Method
log10ws	-7.12		Crippen Method
logp	6.599		Crippen Method
mcvol	353.040	ml/mol	McGowan Method
pc	953.19	kPa	Joback Method
rinsol	2745.00		NIST Webbook
tb	912.75	K	Joback Method
tc	1119.39	K	Joback Method
tf	510.12	K	Joback Method
vc	1.349	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1218.73	J/molxK	912.75	Joback Method
cpg	1238.47	J/molxK	947.19	Joback Method
cpg	1256.66	J/molxK	981.63	Joback Method
cpg	1273.36	J/molxK	1016.07	Joback Method
cpg	1288.61	J/molxK	1050.51	Joback Method
cpg	1302.46	J/molxK	1084.95	Joback Method
cpg	1314.96	J/molxK	1119.39	Joback Method
dvisc	0.0005950	Paxs	510.12	Joback Method
dvisc	0.0002727	Paxs	577.23	Joback Method

dvisc	0.0001470	Paxs	644.33	Joback Method
dvisc	0.0000891	Paxs	711.43	Joback Method
dvisc	0.0000588	Paxs	778.54	Joback Method
dvisc	0.0000415	Paxs	845.64	Joback Method
dvisc	0.0000308	Paxs	912.75	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U367486&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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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