

Diethylmalonic acid, hept-4-yl undecyl ester

Inchi:	InChI=1S/C25H48O4/c1-6-11-12-13-14-15-16-17-18-21-28-23(26)25(9-4,10-5)24(27)29-
InchiKey:	CFKHKMKXJPIHOLS-UHFFFAOYSA-N
Formula:	C25H48O4
SMILES:	CCCCCCCCCOC(=O)C(CC)(CC)C(=O)OC(CCC)CCC
Mol. weight [g/mol]:	412.65

Physical Properties

Property code	Value	Unit	Source
gf	-307.82	kJ/mol	Joback Method
hf	-1062.96	kJ/mol	Joback Method
hfus	55.14	kJ/mol	Joback Method
hvap	87.87	kJ/mol	Joback Method
log10ws	-7.88		Crippen Method
logp	7.379		Crippen Method
mcvol	377.990	ml/mol	McGowan Method
pc	816.79	kPa	Joback Method
rinsol	2431.00		NIST Webbook
tb	920.31	K	Joback Method
tc	1127.45	K	Joback Method
tf	503.25	K	Joback Method
vc	1.466	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1281.45	J/molxK	920.31	Joback Method
cpg	1301.73	J/molxK	954.83	Joback Method
cpg	1320.61	J/molxK	989.36	Joback Method
cpg	1338.12	J/molxK	1023.88	Joback Method
cpg	1354.33	J/molxK	1058.41	Joback Method
cpg	1369.31	J/molxK	1092.93	Joback Method
cpg	1383.09	J/molxK	1127.45	Joback Method
dvisc	0.0004880	Paxs	503.25	Joback Method
dvisc	0.0002009	Paxs	572.76	Joback Method

dvisc	0.0001003	Paxs	642.27	Joback Method
dvisc	0.0000573	Paxs	711.78	Joback Method
dvisc	0.0000362	Paxs	781.29	Joback Method
dvisc	0.0000246	Paxs	850.80	Joback Method
dvisc	0.0000178	Paxs	920.31	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=U370514&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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