

Diethylmalonic acid, phenethyl tetradecyl ester

Inchi:	InChI=1S/C29H48O4/c1-4-7-8-9-10-11-12-13-14-15-16-20-24-32-27(30)29(5-2,6-3)28(31)
InchiKey:	JGLQMVQIJLZBQX-UHFFFAOYSA-N
Formula:	C29H48O4
SMILES:	CCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCCc1ccccc1
Mol. weight [g/mol]:	460.69

Physical Properties

Property code	Value	Unit	Source
gf	-159.29	kJ/mol	Joback Method
hf	-903.71	kJ/mol	Joback Method
hfus	63.07	kJ/mol	Joback Method
hvap	99.44	kJ/mol	Joback Method
log10ws	-8.55		Crippen Method
logp	7.823		Crippen Method
mcvol	410.590	ml/mol	McGowan Method
pc	789.04	kPa	Joback Method
rinpol	3064.00		NIST Webbook
tb	1038.95	K	Joback Method
tc	1276.31	K	Joback Method
tf	589.75	K	Joback Method
vc	1.589	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1433.59	J/molxK	1038.95	Joback Method
cpg	1452.33	J/molxK	1078.51	Joback Method
cpg	1469.46	J/molxK	1118.07	Joback Method
cpg	1485.09	J/molxK	1157.63	Joback Method
cpg	1499.34	J/molxK	1197.19	Joback Method
cpg	1512.31	J/molxK	1236.75	Joback Method
cpg	1524.12	J/molxK	1276.31	Joback Method
dvisc	0.0002030	Paxs	589.75	Joback Method
dvisc	0.0000936	Paxs	664.62	Joback Method

dvisc	0.0000505	Paxs	739.48	Joback Method
dvisc	0.0000305	Paxs	814.35	Joback Method
dvisc	0.0000201	Paxs	889.22	Joback Method
dvisc	0.0000141	Paxs	964.08	Joback Method
dvisc	0.0000104	Paxs	1038.95	Joback Method

Sources

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=U369557&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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