

Diethylmalonic acid, tridecyl 2,4,4-trimethylpentyl ester

Inchi:	InChI=1S/C28H54O4/c1-8-11-12-13-14-15-16-17-18-19-20-21-31-25(29)28(9-2,10-3)26(
InchiKey:	PQCWMFLUCYBXFQ-UHFFFAOYSA-N
Formula:	C28H54O4
SMILES:	CCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCC(C)CC(C)(C)C
Mol. weight [g/mol]:	454.73

Physical Properties

Property code	Value	Unit	Source
gf	-279.72	kJ/mol	Joback Method
hf	-1133.63	kJ/mol	Joback Method
hfus	55.50	kJ/mol	Joback Method
hvap	93.25	kJ/mol	Joback Method
log10ws	-8.54		Crippen Method
logp	8.263		Crippen Method
mvol	420.260	ml/mol	McGowan Method
pc	704.33	kPa	Joback Method
rinpol	2713.00		NIST Webbook
tb	985.72	K	Joback Method
tc	1211.79	K	Joback Method
tf	539.48	K	Joback Method
vc	1.623	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1474.01	J/molxK	985.72	Joback Method
cpg	1495.61	J/molxK	1023.40	Joback Method
cpg	1515.64	J/molxK	1061.08	Joback Method
cpg	1534.22	J/molxK	1098.75	Joback Method
cpg	1551.46	J/molxK	1136.43	Joback Method
cpg	1567.46	J/molxK	1174.11	Joback Method
cpg	1582.33	J/molxK	1211.79	Joback Method
dvisc	0.0002800	Paxs	539.48	Joback Method
dvisc	0.0001090	Paxs	613.85	Joback Method

dvisc	0.0000520	Paxs	688.23	Joback Method
dvisc	0.0000287	Paxs	762.60	Joback Method
dvisc	0.0000176	Paxs	836.97	Joback Method
dvisc	0.0000117	Paxs	911.35	Joback Method
dvisc	0.0000082	Paxs	985.72	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369485&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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