

Diethylmalonic acid, dodecyl 2-isopropylphenyl ester

Inchi:	InChI=1S/C28H46O4/c1-6-9-10-11-12-13-14-15-16-19-22-31-26(29)28(7-2,8-3)27(30)32
InchiKey:	PCYMJGFTWOHMMX-UHFFFAOYSA-N
Formula:	C28H46O4
SMILES:	CCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccccc1C(C)C
Mol. weight [g/mol]:	446.66

Physical Properties

Property code	Value	Unit	Source
gf	-179.78	kJ/mol	Joback Method
hf	-899.82	kJ/mol	Joback Method
hfus	56.57	kJ/mol	Joback Method
hvap	97.49	kJ/mol	Joback Method
log10ws	-8.71		Crippen Method
logp	7.986		Crippen Method
mcvol	396.500	ml/mol	McGowan Method
pc	830.02	kPa	Joback Method
rinpol	2822.00		NIST Webbook
tb	1020.61	K	Joback Method
tc	1250.70	K	Joback Method
tf	576.00	K	Joback Method
vc	1.526	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1369.73	J/molxK	1020.61	Joback Method
cpg	1445.19	J/molxK	1212.35	Joback Method
cpg	1432.88	J/molxK	1174.00	Joback Method
cpg	1419.26	J/molxK	1135.65	Joback Method
cpg	1404.26	J/molxK	1097.31	Joback Method
cpg	1387.78	J/molxK	1058.96	Joback Method
cpg	1456.30	J/molxK	1250.70	Joback Method
dvisc	0.0000114	Paxs	1020.61	Joback Method
dvisc	0.0000155	Paxs	946.51	Joback Method

dvisc	0.0000220	Paxs	872.41	Joback Method
dvisc	0.0000335	Paxs	798.31	Joback Method
dvisc	0.0000556	Paxs	724.20	Joback Method
dvisc	0.0001033	Paxs	650.10	Joback Method
dvisc	0.0002256	Paxs	576.00	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369977&Units=SI

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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