

Diethylmalonic acid, 2-isopropylphenyl octadecyl ester

Inchi:	InChI=1S/C34H58O4/c1-6-9-10-11-12-13-14-15-16-17-18-19-20-21-22-25-28-37-32(35)3
InchiKey:	OAWVYTGOZSKIMX-UHFFFAOYSA-N
Formula:	C34H58O4
SMILES:	CCCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccccc1C(C)C
Mol. weight [g/mol]:	530.82

Physical Properties

Property code	Value	Unit	Source
gf	-129.26	kJ/mol	Joback Method
hf	-1023.66	kJ/mol	Joback Method
hfus	72.11	kJ/mol	Joback Method
hvap	110.84	kJ/mol	Joback Method
log10ws	-11.22		Crippen Method
logp	10.327		Crippen Method
mvol	481.040	ml/mol	McGowan Method
pc	610.57	kPa	Joback Method
rinpol	3454.00		NIST Webbook
rinpol	3454.00		NIST Webbook
tb	1157.89	K	Joback Method
tc	1453.05	K	Joback Method
tf	643.62	K	Joback Method
vc	1.863	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1755.10	J/molxK	1157.89	Joback Method
cpg	1776.16	J/molxK	1207.08	Joback Method
cpg	1794.88	J/molxK	1256.28	Joback Method
cpg	1811.51	J/molxK	1305.47	Joback Method
cpg	1826.28	J/molxK	1354.66	Joback Method
cpg	1839.44	J/molxK	1403.86	Joback Method
cpg	1851.24	J/molxK	1453.05	Joback Method
dvisc	0.0000952	Paxs	643.62	Joback Method

dvisc	0.0000418	Paxs	729.33	Joback Method
dvisc	0.0000218	Paxs	815.04	Joback Method
dvisc	0.0000129	Paxs	900.75	Joback Method
dvisc	0.0000083	Paxs	986.47	Joback Method
dvisc	0.0000058	Paxs	1072.18	Joback Method
dvisc	0.0000042	Paxs	1157.89	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369983&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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