

Sebacic acid, ethyl 4-phenylphenyl ester

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C24H30O4/c1-2-27-23(25)14-10-5-3-4-6-11-15-24(26)28-22-18-16-21(17-19-20)30-29

KQUCSNQZHHUO-UHFFFAOYSA-N

C24H30O4

CCOC(=O)CCCCCCCCC(=O)Oc1ccc(-c2ccccc2)cc1

382.49

Physical Properties

Property code	Value	Unit	Source
gf	-101.45	kJ/mol	Joback Method
hf	-566.70	kJ/mol	Joback Method
hfus	51.18	kJ/mol	Joback Method
hvap	92.54	kJ/mol	Joback Method
log10ws	-7.44		Crippen Method
logp	5.943		Crippen Method
mcvol	316.380	ml/mol	McGowan Method
pc	1291.14	kPa	Joback Method
rinpol	3152.00		NIST Webbook
rinpol	3152.00		NIST Webbook
tb	959.44	K	Joback Method
tc	1182.13	K	Joback Method
tf	569.92	K	Joback Method
vc	1.212	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1016.74	J/mol×K	959.44	Joback Method
cpg	1075.71	J/mol×K	1145.01	Joback Method
cpg	1066.47	J/mol×K	1107.90	Joback Method
cpg	1056.00	J/mol×K	1070.78	Joback Method
cpg	1044.26	J/mol×K	1033.67	Joback Method
cpg	1031.19	J/mol×K	996.55	Joback Method
cpg	1083.79	J/mol×K	1182.13	Joback Method
dvisc	0.0000318	Pa×s	959.44	Joback Method

dvisc	0.0000409	Pa×s	894.52	Joback Method
dvisc	0.0000547	Pa×s	829.60	Joback Method
dvisc	0.0000768	Pa×s	764.68	Joback Method
dvisc	0.0001149	Pa×s	699.76	Joback Method
dvisc	0.0001867	Pa×s	634.84	Joback Method
dvisc	0.0003390	Pa×s	569.92	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U355249&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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