

Fumaric acid, 4-phenylphenyl undecyl ester

Inchi: InChI=1S/C27H34O4/c1-2-3-4-5-6-7-8-9-13-22-30-26(28)20-21-27(29)31-25-18-16-24(17)
InchiKey: PCXNPXFWWRYTR-QZQOTICOSA-N
Formula: C27H34O4
SMILES: CCCCCCCCCCOC(=O)C=CC(=O)Oc1ccc(-c2ccccc2)cc1
Mol. weight [g/mol]: 422.56

Physical Properties

Property code	Value	Unit	Source
gf	4.03	kJ/mol	Joback Method
hf	-511.40	kJ/mol	Joback Method
hfus	59.15	kJ/mol	Joback Method
hvap	99.18	kJ/mol	Joback Method
log10ws	-8.55		Crippen Method
logp	6.889		Crippen Method
mcvol	354.350	ml/mol	McGowan Method
pc	1097.17	kPa	Joback Method
rinqol	3495.00		NIST Webbook
tb	1032.24	K	Joback Method
tc	1264.91	K	Joback Method
tf	598.65	K	Joback Method
vc	1.359	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1169.92	J/molxK	1032.24	Joback Method
cpg	1184.59	J/molxK	1071.02	Joback Method
cpg	1197.92	J/molxK	1109.80	Joback Method
cpg	1210.01	J/molxK	1148.57	Joback Method
cpg	1220.95	J/molxK	1187.35	Joback Method
cpg	1230.83	J/molxK	1226.13	Joback Method
cpg	1239.74	J/molxK	1264.91	Joback Method
dvisc	0.0002203	Paxs	598.65	Joback Method
dvisc	0.0001156	Paxs	670.92	Joback Method

dvisc	0.0000688	Paxs	743.18	Joback Method
dvisc	0.0000449	Paxs	815.45	Joback Method
dvisc	0.0000314	Paxs	887.71	Joback Method
dvisc	0.0000232	Paxs	959.98	Joback Method
dvisc	0.0000179	Paxs	1032.24	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=U348217&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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