

Fumaric acid, 4-methoxyphenyl naphth-2-ylmethyl ester

Inchi:	InChI=1S/C22H18O5/c1-25-19-8-10-20(11-9-19)27-22(24)13-12-21(23)26-15-16-6-7-17-
InchiKey:	UFCUGCDPDVEOQA-OUKQBFOZSA-N
Formula:	C22H18O5
SMILES:	COc1ccc(OC(=O)C=CC(=O)OCc2ccc3ccccc3c2)cc1
Mol. weight [g/mol]:	362.38

Physical Properties

Property code	Value	Unit	Source
gf	-46.05	kJ/mol	Joback Method
hf	-360.82	kJ/mol	Joback Method
hfus	44.02	kJ/mol	Joback Method
hvap	92.76	kJ/mol	Joback Method
log10ws	-5.79		Crippen Method
logp	4.053		Crippen Method
mcvol	270.310	ml/mol	McGowan Method
pc	1848.33	kPa	Joback Method
rinpol	3139.00		NIST Webbook
tb	964.22	K	Joback Method
tc	1207.66	K	Joback Method
tf	609.75	K	Joback Method
vc	1.020	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	812.95	J/molxK	964.22	Joback Method
cpg	824.70	J/molxK	1004.79	Joback Method
cpg	835.28	J/molxK	1045.37	Joback Method
cpg	844.77	J/molxK	1085.94	Joback Method
cpg	853.25	J/molxK	1126.51	Joback Method
cpg	860.80	J/molxK	1167.09	Joback Method
cpg	867.50	J/molxK	1207.66	Joback Method
dvisc	0.0003347	Paxs	609.75	Joback Method
dvisc	0.0002204	Paxs	668.83	Joback Method

dvisc	0.0001554	Paxs	727.91	Joback Method
dvisc	0.0001154	Paxs	786.99	Joback Method
dvisc	0.0000893	Paxs	846.06	Joback Method
dvisc	0.0000715	Paxs	905.14	Joback Method
dvisc	0.0000588	Paxs	964.22	Joback Method

Sources

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=U405786&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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