

Fumaric acid, di(naphth-2-yl) ester

Inchi:	InChI=1S/C24H16O4/c25-23(27-21-11-9-17-5-1-3-7-19(17)15-21)13-14-24(26)28-22-12-
InchiKey:	OQTWKMMWTVVXPX-BUHFOSPRSA-N
Formula:	C24H16O4
SMILES:	O=C(C=CC(=O)Oc1ccc2ccccc2c1)Oc1ccc2ccccc2c1
Mol. weight [g/mol]:	368.38

Physical Properties

Property code	Value	Unit	Source
gf	182.44	kJ/mol	Joback Method
hf	-78.81	kJ/mol	Joback Method
hfus	45.03	kJ/mol	Joback Method
hvap	96.44	kJ/mol	Joback Method
log10ws	-7.21		Crippen Method
logp	5.060		Crippen Method
mvol	273.160	ml/mol	McGowan Method
pc	1964.82	kPa	Joback Method
rinpol	3347.00		NIST Webbook
tb	1006.54	K	Joback Method
tc	1265.54	K	Joback Method
tf	642.76	K	Joback Method
vc	1.036	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	819.18	J/molxK	1006.54	Joback Method
cpg	831.34	J/molxK	1049.71	Joback Method
cpg	842.82	J/molxK	1092.87	Joback Method
cpg	853.79	J/molxK	1136.04	Joback Method
cpg	864.43	J/molxK	1179.21	Joback Method
cpg	874.90	J/molxK	1222.37	Joback Method
cpg	885.39	J/molxK	1265.54	Joback Method
dvisc	0.0005651	Paxs	642.76	Joback Method
dvisc	0.0003960	Paxs	703.39	Joback Method

dvisc	0.0002936	Paxs	764.02	Joback Method
dvisc	0.0002274	Paxs	824.65	Joback Method
dvisc	0.0001825	Paxs	885.28	Joback Method
dvisc	0.0001506	Paxs	945.91	Joback Method
dvisc	0.0001272	Paxs	1006.54	Joback Method

Sources

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=U405839&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
mccvol:	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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