

Fumaric acid, naphth-2-yl dec-2-yl ester

Inchi:	InChI=1S/C24H30O4/c1-3-4-5-6-7-8-11-19(2)27-23(25)16-17-24(26)28-22-15-14-20-12-9
InchiKey:	PHBKMCCQTGKZJKC-WUKNDPDISA-N
Formula:	C24H30O4
SMILES:	CCCCCCCCC(C)OC(=O)C=CC(=O)Oc1ccc2ccccc2c1
Mol. weight [g/mol]:	382.49

Physical Properties

Property code	Value	Unit	Source
gf	-29.43	kJ/mol	Joback Method
hf	-500.22	kJ/mol	Joback Method
hfus	50.84	kJ/mol	Joback Method
hvap	91.48	kJ/mol	Joback Method
log10ws	-7.44		Crippen Method
logp	5.984		Crippen Method
mvol	316.380	ml/mol	McGowan Method
pc	1267.35	kPa	Joback Method
rinpol	3002.00		NIST Webbook
rinpol	3002.00		NIST Webbook
tb	955.46	K	Joback Method
tc	1176.79	K	Joback Method
tf	556.12	K	Joback Method
vc	1.216	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1011.97	J/molxK	955.46	Joback Method
cpg	1027.15	J/molxK	992.35	Joback Method
cpg	1041.26	J/molxK	1029.24	Joback Method
cpg	1054.39	J/molxK	1066.13	Joback Method
cpg	1066.62	J/molxK	1103.01	Joback Method
cpg	1078.04	J/molxK	1139.90	Joback Method
cpg	1088.73	J/molxK	1176.79	Joback Method
dvisc	0.0004862	Paxs	556.12	Joback Method

dvisc	0.0002729	Paxs	622.68	Joback Method
dvisc	0.0001712	Paxs	689.23	Joback Method
dvisc	0.0001166	Paxs	755.79	Joback Method
dvisc	0.0000845	Paxs	822.35	Joback Method
dvisc	0.0000643	Paxs	888.90	Joback Method
dvisc	0.0000508	Paxs	955.46	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=U405833&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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