Fumaric acid, monoamide, N,N-dimethyl-, 1-naphthyl ester

Inchi: InChI=1S/C16H15NO3/c1-17(2)15(18)10-11-16(19)20-14-9-5-7-12-6-3-4-8-13(12)14/h3-1

InchiKey: LMABEVZVSHRUTH-ZHACJKMWSA-N

Formula: C16H15NO3

SMILES: CN(C)C(=O)C=CC(=O)Oc1cccc2ccccc12

Mol. weight [g/mol]: 269.30

Physical Properties

Property code	Value	Unit	Source
gf	121.43	kJ/mol	Joback Method
hf	-130.07	kJ/mol	Joback Method
hfus	35.48	kJ/mol	Joback Method
hvap	73.69	kJ/mol	Joback Method
log10ws	-3.46		Crippen Method
logp	2.390		Crippen Method
mcvol	207.770	ml/mol	McGowan Method
pc	2417.12	kPa	Joback Method
rinpol	2627.00		NIST Webbook
tb	762.88	K	Joback Method
tc	991.96	K	Joback Method
tf	491.20	K	Joback Method
vc	0.773	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	567.36	J/mol×K	762.88	Joback Method
cpg	580.73	J/mol×K	801.06	Joback Method
cpg	593.10	J/mol×K	839.24	Joback Method
cpg	604.58	J/mol×K	877.42	Joback Method
cpg	615.25	J/mol×K	915.60	Joback Method
cpg	625.20	J/mol×K	953.78	Joback Method
cpg	634.53	J/mol×K	991.96	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=U357437&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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