Fumaric acid, monoamide, N-methyl-N-phenyl-, 1-naphthyl ester

Inchi: InChI=1S/C21H17NO3/c1-22(17-10-3-2-4-11-17)20(23)14-15-21(24)25-19-13-7-9-16-8-5

InchiKey: LEALJGJJNFWDDP-CCEZHUSRSA-N

Formula: C21H17NO3

SMILES: CN(C(=O)C=CC(=O)Oc1cccc2ccccc12)c1ccccc1

Mol. weight [g/mol]: 331.36

Physical Properties

Property code	Value	Unit	Source
gf	275.94	kJ/mol	Joback Method
hf	3.26	kJ/mol	Joback Method
hfus	42.47	kJ/mol	Joback Method
hvap	87.10	kJ/mol	Joback Method
log10ws	-5.19		Crippen Method
logp	3.964		Crippen Method
mcvol	254.460	ml/mol	McGowan Method
pc	2098.42	kPa	Joback Method
rinpol	3108.00		NIST Webbook
tb	903.96	K	Joback Method
tc	1151.00	K	Joback Method
tf	573.97	K	Joback Method
vc	0.946	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	746.70	J/mol×K	903.96	Joback Method
cpg	759.83	J/mol×K	945.13	Joback Method
cpg	771.99	J/mol×K	986.31	Joback Method
cpg	783.34	J/mol×K	1027.48	Joback Method
cpg	794.03	J/mol×K	1068.65	Joback Method
cpg	804.21	J/mol×K	1109.82	Joback Method
cpg	814.02	J/mol×K	1151.00	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=U357438&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
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