Fumaric acid, monoamide, N,N-dimethyl-, 4-(2-phenylprop-2yl)phenyl ester

Inchi: InChI=1S/C21H23NO3/c1-21(2,16-8-6-5-7-9-16)17-10-12-18(13-11-17)25-20(24)15-14-1

InchiKey: DTHOVJNLXLMMPO-CCEZHUSRSA-N

Formula: C21H23NO3

SMILES: CN(C)C(=O)C=CC(=O)Oc1ccc(C(C)(C)c2ccccc2)cc1

Mol. weight [g/mol]: 337.41

Physical Properties

Property code	Value	Unit	Source
gf	172.13	kJ/mol	Joback Method
hf	-196.56	kJ/mol	Joback Method
hfus	38.03	kJ/mol	Joback Method
hvap	84.16	kJ/mol	Joback Method
log10ws	-4.27		Crippen Method
logp	3.562		Crippen Method
mcvol	273.920	ml/mol	McGowan Method
pc	1723.16	kPa	Joback Method
rinpol	3066.00		NIST Webbook
tb	881.75	K	Joback Method
tc	1117.77	K	Joback Method
tf	543.69	K	Joback Method
vc	1.012	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	826.79	J/mol×K	881.75	Joback Method
cpg	841.64	J/mol×K	921.09	Joback Method
cpg	855.34	J/mol×K	960.42	Joback Method
cpg	868.02	J/mol×K	999.76	Joback Method
cpg	879.82	J/mol×K	1039.09	Joback Method
cpg	890.84	J/mol×K	1078.43	Joback Method
cpg	901.23	J/mol×K	1117.77	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U357413&Units=SI

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