Fumaric acid, monoamide, N,N-dimethyl-, 2,6-dichlorophenyl ester

Inchi: InChI=1S/C12H11Cl2NO3/c1-15(2)10(16)6-7-11(17)18-12-8(13)4-3-5-9(12)14/h3-7H,1-2

InchiKey: IDKXXNKHJUIKRA-VOTSOKGWSA-N

Formula: C12H11Cl2NO3

SMILES: CN(C)C(=O)C=CC(=O)Oc1c(Cl)cccc1Cl

Mol. weight [g/mol]: 288.13

Physical Properties

Property code	Value	Unit	Source
gf	-52.39	kJ/mol	Joback Method
hf	-281.53	kJ/mol	Joback Method
hfus	36.10	kJ/mol	Joback Method
hvap	72.58	kJ/mol	Joback Method
log10ws	-3.03		Crippen Method
logp	2.543		Crippen Method
mcvol	195.350	ml/mol	McGowan Method
pc	2540.49	kPa	Joback Method
rinpol	2305.00		NIST Webbook
rinpol	2305.00		NIST Webbook
tb	732.22	K	Joback Method
tc	958.69	K	Joback Method
tf	485.78	K	Joback Method
vc	0.726	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	472.66	J/mol×K	732.22	Joback Method
cpg	483.71	J/mol×K	769.97	Joback Method
cpg	493.92	J/mol×K	807.71	Joback Method
cpg	503.32	J/mol×K	845.46	Joback Method
cpg	511.95	J/mol×K	883.20	Joback Method
cpg	519.87	J/mol×K	920.95	Joback Method
cpg	527.12	J/mol×K	958.69	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=U357445&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