Fumaric acid, monoamide, N,N-dimethyl-, 4-chloro-3-methylphenyl ester

Inchi: InChI=1S/C13H14ClNO3/c1-9-8-10(4-5-11(9)14)18-13(17)7-6-12(16)15(2)3/h4-8H,1-3H3

InchiKey: HRZDMAGODUSSFJ-VOTSOKGWSA-N

Formula: C13H14ClNO3

SMILES: Cc1cc(OC(=O)C=CC(=O)N(C)C)ccc1Cl

Mol. weight [g/mol]: 267.71

Physical Properties

Property code	Value	Unit	Source
gf	-32.04	kJ/mol	Joback Method
hf	-286.43	kJ/mol	Joback Method
hfus	34.49	kJ/mol	Joback Method
hvap	70.42	kJ/mol	Joback Method
log10ws	-2.82		Crippen Method
logp	2.198		Crippen Method
mcvol	197.200	ml/mol	McGowan Method
pc	2395.87	kPa	Joback Method
rinpol	2340.00		NIST Webbook
rinpol	2340.00		NIST Webbook
tb	717.67	K	Joback Method
tc	937.62	K	Joback Method
tf	467.13	K	Joback Method
vc	0.733	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	501.24	J/mol×K	717.67	Joback Method
cpg	513.89	J/mol×K	754.33	Joback Method
cpg	525.64	J/mol×K	790.99	Joback Method
cpg	536.55	J/mol×K	827.65	Joback Method
cpg	546.64	J/mol×K	864.31	Joback Method
cpg	555.97	J/mol×K	900.97	Joback Method
cpg	564.57	J/mol×K	937.62	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=U357440&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

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