

Fumaric acid, monoamide, N-(2-ethylphenyl)-, 3,5-difluorophenyl ester

Other names:	Fumaric acid, monoamide, N-(2-ethylphenyl)-, 3,5-fluorophenyl ester
Inchi:	InChI=1S/C18H15F2NO3/c1-2-12-5-3-4-6-16(12)21-17(22)7-8-18(23)24-15-10-13(19)9-1
InchiKey:	ZHYKIZJDNAKQTO-BQYQJAHWSA-N
Formula:	C18H15F2NO3
SMILES:	CCc1ccccc1NC(=O)C=CC(=O)Oc1cc(F)cc(F)c1
Mol. weight [g/mol]:	331.31

Physical Properties

Property code	Value	Unit	Source
gf	-286.24	kJ/mol	Joback Method
hf	-555.11	kJ/mol	Joback Method
hfus	45.14	kJ/mol	Joback Method
hvap	82.86	kJ/mol	Joback Method
log10ws	-4.96		Crippen Method
logp	3.627		Crippen Method
mcvol	235.190	ml/mol	McGowan Method
pc	1984.12	kPa	Joback Method
rinpol	2609.00		NIST Webbook
tb	862.57	K	Joback Method
tc	1086.06	K	Joback Method
tf	553.87	K	Joback Method
vc	0.908	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	679.86	J/molxK	862.57	Joback Method
cpg	691.71	J/molxK	899.82	Joback Method
cpg	702.56	J/molxK	937.07	Joback Method
cpg	712.47	J/molxK	974.32	Joback Method
cpg	721.49	J/molxK	1011.57	Joback Method
cpg	729.67	J/molxK	1048.82	Joback Method
cpg	737.08	J/molxK	1086.06	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357407&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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