

1,2-Cyclohexanedicarboxylic acid, 2-fluorophenyl isobutyl ester

Inchi:	InChI=1S/C18H23FO4/c1-12(2)11-22-17(20)13-7-3-4-8-14(13)18(21)23-16-10-6-5-9-15(
InchiKey:	SXFDBFSFIRVAMI-UHFFFAOYSA-N
Formula:	C18H23FO4
SMILES:	CC(C)COC(=O)C1CCCCC1C(=O)Oc1ccccc1F
Mol. weight [g/mol]:	322.37

Physical Properties

Property code	Value	Unit	Source
gf	-444.89	kJ/mol	Joback Method
hf	-846.80	kJ/mol	Joback Method
hfus	34.06	kJ/mol	Joback Method
hvap	75.83	kJ/mol	Joback Method
log10ws	-4.33		Crippen Method
logp	3.737		Crippen Method
mcvol	246.510	ml/mol	McGowan Method
pc	1731.78	kPa	Joback Method
rinpol	2163.00		NIST Webbook
tb	809.19	K	Joback Method
tc	1028.13	K	Joback Method
tf	464.61	K	Joback Method
vc	0.927	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	767.51	J/molxK	809.19	Joback Method
cpg	784.56	J/molxK	845.68	Joback Method
cpg	800.15	J/molxK	882.17	Joback Method
cpg	814.31	J/molxK	918.66	Joback Method
cpg	827.05	J/molxK	955.15	Joback Method
cpg	838.38	J/molxK	991.64	Joback Method
cpg	848.33	J/molxK	1028.13	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339780&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
mccvol:	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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