

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

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

Physical Properties

Property code	Value	Unit	Source
gf	-442.45	kJ/mol	Joback Method
hf	-841.52	kJ/mol	Joback Method
hfus	37.59	kJ/mol	Joback Method
hvap	76.22	kJ/mol	Joback Method
log10ws	-4.58		Crippen Method
logp	3.881		Crippen Method
mcvol	246.510	ml/mol	McGowan Method
pc	1720.31	kPa	Joback Method
tb	809.63	K	Joback Method
tc	1025.48	K	Joback Method
tf	479.61	K	Joback Method
vc	0.933	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	766.97	J/molxK	809.63	Joback Method
cpg	783.79	J/molxK	845.60	Joback Method
cpg	799.21	J/molxK	881.58	Joback Method
cpg	813.23	J/molxK	917.55	Joback Method
cpg	825.89	J/molxK	953.53	Joback Method
cpg	837.20	J/molxK	989.50	Joback Method
cpg	847.17	J/molxK	1025.48	Joback Method

Sources

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=U339781&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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