Fumaric acid, 4-cyanophenyl cyclohexylmethyl ester

Inchi: InChI=1S/C18H19NO4/c19-12-14-6-8-16(9-7-14)23-18(21)11-10-17(20)22-13-15-4-2-1-3

InchiKey: PSFQKRQWOREWNQ-ZHACJKMWSA-N

Formula: C18H19NO4

SMILES: N#Cc1ccc(OC(=O)C=CC(=O)OCC2CCCCC2)cc1

Mol. weight [g/mol]: 313.35

Physical Properties

Property code	Value	Unit	Source
gf	-26.53	kJ/mol	Joback Method
hf	-342.97	kJ/mol	Joback Method
hfus	35.14	kJ/mol	Joback Method
hvap	87.78	kJ/mol	Joback Method
log10ws	-4.27		Crippen Method
logp	3.143		Crippen Method
mcvol	241.820	ml/mol	McGowan Method
pc	1880.53	kPa	Joback Method
rinpol	2602.00		NIST Webbook
rinpol	2602.00		NIST Webbook
tb	921.27	K	Joback Method
tc	1162.07	K	Joback Method
tf	543.17	K	Joback Method
vc	0.922	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	749.17	J/mol×K	921.27	Joback Method
cpg	761.68	J/mol×K	961.40	Joback Method
cpg	772.81	J/mol×K	1001.54	Joback Method
cpg	782.61	J/mol×K	1041.67	Joback Method
cpg	791.13	J/mol×K	1081.81	Joback Method
cpg	798.41	J/mol×K	1121.94	Joback Method
cpg	804.51	J/mol×K	1162.07	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=U405732&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