Fumaric acid, 2-nitrophenyl cyclohexylmethyl ester

Inchi: InChI=1S/C17H19NO6/c19-16(23-12-13-6-2-1-3-7-13)10-11-17(20)24-15-9-5-4-8-14(15)

InchiKey: QEJAUIYGUWHNKR-ZHACJKMWSA-N

Formula: C17H19NO6

SMILES: O=C(C=CC(=O)Oc1ccccc1[N+](=O)[O-])OCC1CCCCC1

Mol. weight [g/mol]: 333.34

Physical Properties

Property code	Value	Unit	Source
gf	-132.58	kJ/mol	Joback Method
hf	-497.97	kJ/mol	Joback Method
hfus	42.41	kJ/mol	Joback Method
hvap	91.66	kJ/mol	Joback Method
log10ws	-4.57		Crippen Method
logp	3.180		Crippen Method
mcvol	243.770	ml/mol	McGowan Method
pc	2117.78	kPa	Joback Method
rinpol	2644.00		NIST Webbook
rinpol	2644.00		NIST Webbook
tb	948.15	K	Joback Method
tc	1198.80	K	Joback Method
tf	610.52	K	Joback Method
vc	0.922	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	775.72	J/mol×K	948.15	Joback Method
cpg	787.87	J/mol×K	989.92	Joback Method
cpg	798.52	J/mol×K	1031.70	Joback Method
cpg	807.72	J/mol×K	1073.47	Joback Method
cpg	815.55	J/mol×K	1115.25	Joback Method
cpg	822.05	J/mol×K	1157.02	Joback Method
cpg	827.30	J/mol×K	1198.80	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405797&Units=SI
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

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