Fumaric acid, 4-octyl cyclohexylmethyl ester

Inchi: InChI=1S/C19H32O4/c1-3-5-12-17(9-4-2)23-19(21)14-13-18(20)22-15-16-10-7-6-8-11-16
InchiKey: NPENSVNRKVAMOR-BUHFOSPRSA-N
Formula: C19H32O4
SMILES: CCCCC(CCC)OC(=O)C=CC(=O)OCC1CCCCC1
Mol. weight [g/mol]: 324.45

Physical Properties

Property code	Value	Unit	Source
gf	-256.51	kJ/mol	Joback Method
hf	-758.83	kJ/mol	Joback Method
hfus	39.05	kJ/mol	Joback Method
hvap	76.20	kJ/mol	Joback Method
log10ws	-5.12		Crippen Method
logp	4.568		Crippen Method
mcvol	278.290	ml/mol	McGowan Method
pc	1387.11	kPa	Joback Method
rinpol	2241.00		NIST Webbook
rinpol	2241.00		NIST Webbook
tb	809.97	K	Joback Method
tc	1011.57	K	Joback Method
tf	435.51	K	Joback Method
vc	1.054	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	880.96	J/mol×K	809.97	Joback Method
cpg	961.26	J/mol×K	977.97	Joback Method
cpg	947.58	J/mol×K	944.37	Joback Method
cpg	932.74	J/mol×K	910.77	Joback Method
cpg	916.71	J/mol×K	877.17	Joback Method
cpg	899.46	J/mol×K	843.57	Joback Method
cpg	973.83	J/mol×K	1011.57	Joback Method
dvisc	0.0000508	Pa×s	809.97	Joback Method

dvisc	0.0000690	Pa×s	747.56	Joback Method
dvisc	0.0000992	Pa×s	685.15	Joback Method
dvisc	0.0001532	Pa×s	622.74	Joback Method
dvisc	0.0002608	Pa×s	560.33	Joback Method
dvisc	0.0005074	Pa×s	497.92	Joback Method
dvisc	0.0011943	Pa×s	435.51	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405623&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
dvisc:	Dynamic viscosity
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