Fumaric acid, 4-octyl naphth-2-ylmethyl ester

Inchi: InChI=1S/C23H28O4/c1-3-5-11-21(8-4-2)27-23(25)15-14-22(24)26-17-18-12-13-19-9-6-7
InchiKey: JUYKHPNSFSYLDH-CCEZHUSRSA-N
Formula: C23H28O4
SMILES: CCCCC(CCC)OC(=O)C=CC(=O)OCc1ccc2ccccc2c1
Mol. weight [g/mol]: 368.47

Physical Properties

Property code	Value	Unit	Source
gf	-37.85	kJ/mol	Joback Method
hf	-479.58	kJ/mol	Joback Method
hfus	48.25	kJ/mol	Joback Method
hvap	89.25	kJ/mol	Joback Method
log10ws	-6.87		Crippen Method
logp	5.341		Crippen Method
mcvol	302.290	ml/mol	McGowan Method
pc	1358.63	kPa	Joback Method
rinpol	2852.00		NIST Webbook
rinpol	2852.00		NIST Webbook
tb	932.58	K	Joback Method
tc	1152.87	K	Joback Method
tf	544.85	K	Joback Method
vc	1.159	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	951.96	J/mol×K	932.58	Joback Method
cpg	966.89	J/mol×K	969.29	Joback Method
cpg	980.77	J/mol×K	1006.01	Joback Method
cpg	993.67	J/mol×K	1042.72	Joback Method
cpg	1005.68	J/mol×K	1079.44	Joback Method
cpg	1016.88	J/mol×K	1116.15	Joback Method
cpg	1027.33	J/mol×K	1152.87	Joback Method
dvisc	0.0005377	Pa×s	544.85	Joback Method

dvisc	0.0003051	Pa×s	609.47	Joback Method
dvisc	0.0001930	Pa×s	674.09	Joback Method
dvisc	0.0001323	Pa×s	738.71	Joback Method
dvisc	0.0000963	Pa×s	803.34	Joback Method
dvisc	0.0000736	Pa×s	867.96	Joback Method
dvisc	0.0000583	Pa×s	932.58	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405628&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

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