

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

Inchi: InChI=1S/C23H28O4/c1-3-4-5-6-9-18(2)27-23(25)15-14-22(24)26-17-19-12-13-20-10-7-8
InchiKey: ZLHWJTGCZWPQAC-CCEZHUSRSA-N
Formula: C23H28O4
SMILES: CCCCCC(C)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
mvol	302.290	ml/mol	McGowan Method
pc	1358.63	kPa	Joback Method
rinpol	2894.00		NIST Webbook
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tb	932.58	K	Joback Method
tc	1152.87	K	Joback Method
tf	544.85	K	Joback Method
vc	1.159	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	951.96	J/molxK	932.58	Joback Method
cpg	1016.88	J/molxK	1116.15	Joback Method
cpg	1005.68	J/molxK	1079.44	Joback Method
cpg	993.67	J/molxK	1042.72	Joback Method
cpg	980.77	J/molxK	1006.01	Joback Method
cpg	966.89	J/molxK	969.29	Joback Method
cpg	1027.33	J/molxK	1152.87	Joback Method
dvisc	0.0000583	Paxs	932.58	Joback Method

dvisc	0.0000736	Paxs	867.96	Joback Method
dvisc	0.0000963	Paxs	803.34	Joback Method
dvisc	0.0001323	Paxs	738.71	Joback Method
dvisc	0.0001930	Paxs	674.09	Joback Method
dvisc	0.0003051	Paxs	609.47	Joback Method
dvisc	0.0005377	Paxs	544.85	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=U405596&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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

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