

Fumaric acid, 3-phenylpropyl naphth-2-ylmethyl ester

Inchi:	InChI=1S/C24H22O4/c25-23(27-16-6-9-19-7-2-1-3-8-19)14-15-24(26)28-18-20-12-13-21
InchiKey:	HSTLOZLMFWXKTN-CCEZHUSRSA-N
Formula:	C24H22O4
SMILES:	O=C(C=CC(=O)OCc1ccc2ccccc2c1)OCCc1cccc1
Mol. weight [g/mol]:	374.43

Physical Properties

Property code	Value	Unit	Source
gf	85.42	kJ/mol	Joback Method
hf	-258.41	kJ/mol	Joback Method
hfus	48.40	kJ/mol	Joback Method
hvap	94.14	kJ/mol	Joback Method
log10ws	-6.28		Crippen Method
logp	4.615		Crippen Method
mvol	292.620	ml/mol	McGowan Method
pc	1618.07	kPa	Joback Method
rinpol	3167.00		NIST Webbook
tb	982.58	K	Joback Method
tc	1223.07	K	Joback Method
tf	597.54	K	Joback Method
vc	1.113	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	905.28	J/molxK	982.58	Joback Method
cpg	961.73	J/molxK	1182.99	Joback Method
cpg	951.99	J/molxK	1142.91	Joback Method
cpg	941.59	J/molxK	1102.82	Joback Method
cpg	930.42	J/molxK	1062.74	Joback Method
cpg	918.35	J/molxK	1022.66	Joback Method
cpg	970.92	J/molxK	1223.07	Joback Method
dvisc	0.0000583	Paxs	982.58	Joback Method
dvisc	0.0000721	Paxs	918.41	Joback Method

dvisc	0.0000922	Paxs	854.23	Joback Method
dvisc	0.0001227	Paxs	790.06	Joback Method
dvisc	0.0001716	Paxs	725.89	Joback Method
dvisc	0.0002563	Paxs	661.71	Joback Method
dvisc	0.0004171	Paxs	597.54	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405674&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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