Fumaric acid, naphth-2-yl 2-methylpent-3-yl ester

Inchi: InChI=1S/C20H22O4/c1-4-18(14(2)3)24-20(22)12-11-19(21)23-17-10-9-15-7-5-6-8-16(15

InchiKey: FRZQWWBZIAFHDU-VAWYXSNFSA-N

Formula: C20H22O4

SMILES: CCC(OC(=O)C=CC(=O)Oc1ccc2ccccc2c1)C(C)C

Mol. weight [g/mol]: 326.39

Physical Properties

Property code	Value	Unit	Source
gf	-65.55	kJ/mol	Joback Method
hf	-422.94	kJ/mol	Joback Method
hfus	36.96	kJ/mol	Joback Method
hvap	82.19	kJ/mol	Joback Method
log10ws	-5.52		Crippen Method
logp	4.279		Crippen Method
mcvol	260.020	ml/mol	McGowan Method
pc	1711.78	kPa	Joback Method
rinpol	2558.00		NIST Webbook
rinpol	2558.00		NIST Webbook
tb	863.50	K	Joback Method
tc	1088.27	K	Joback Method
tf	496.04	K	Joback Method
vc	0.986	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	776.80	J/mol×K	863.50	Joback Method
cpg	791.21	J/mol×K	900.96	Joback Method
cpg	804.55	J/mol×K	938.42	Joback Method
cpg	816.89	J/mol×K	975.89	Joback Method
cpg	828.29	J/mol×K	1013.35	Joback Method
cpg	838.85	J/mol×K	1050.81	Joback Method
cpg	848.61	J/mol×K	1088.27	Joback Method
dvisc	0.0007818	Pa×s	496.04	Joback Method

dvisc	0.0004330	Pa×s	557.28	Joback Method
dvisc	0.0002696	Pa×s	618.53	Joback Method
dvisc	0.0001828	Pa×s	679.77	Joback Method
dvisc	0.0001322	Pa×s	741.01	Joback Method
dvisc	0.0001004	Pa×s	802.26	Joback Method
dvisc	0.0000793	Pa×s	863.50	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405825&Units=SI

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