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

Inchi: InChI=1S/C19H20O4/c1-13(2)14(3)22-18(20)10-11-19(21)23-17-9-8-15-6-4-5-7-16(15)12

InchiKey: AOQROGSMGOYKKL-ZHACJKMWSA-N

Formula: C19H20O4

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

Mol. weight [g/mol]: 312.36

Physical Properties

Property code	Value	Unit	Source
gf	-73.97	kJ/mol	Joback Method
hf	-402.30	kJ/mol	Joback Method
hfus	34.37	kJ/mol	Joback Method
hvap	79.96	kJ/mol	Joback Method
log10ws	-5.11		Crippen Method
logp	3.889		Crippen Method
mcvol	245.930	ml/mol	McGowan Method
pc	1856.31	kPa	Joback Method
rinpol	2472.00		NIST Webbook
tb	840.62	K	Joback Method
tc	1067.69	K	Joback Method
tf	484.77	K	Joback Method
vc	0.929	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	719.87	J/mol×K	840.62	Joback Method
cpg	734.06	J/mol×K	878.47	Joback Method
cpg	747.18	J/mol×K	916.31	Joback Method
cpg	759.30	J/mol×K	954.16	Joback Method
cpg	770.49	J/mol×K	992.00	Joback Method
cpg	780.81	J/mol×K	1029.85	Joback Method
cpg	790.35	J/mol×K	1067.69	Joback Method
dvisc	0.0008518	Pa×s	484.77	Joback Method
dvisc	0.0004777	Pa×s	544.08	Joback Method

dvisc	0.0003001	Pa×s	603.39	Joback Method
dvisc	0.0002049	Pa×s	662.69	Joback Method
dvisc	0.0001490	Pa×s	722.00	Joback Method
dvisc	0.0001137	Pa×s	781.31	Joback Method
dvisc	0.0000901	Pa×s	840.62	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=U405824&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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