Fumaric acid, naphth-1-yl 3-methylbut-2-en-1-yl ester

Inchi: InChI=1S/C19H18O4/c1-14(2)12-13-22-18(20)10-11-19(21)23-17-9-5-7-15-6-3-4-8-16(15

InchiKey: AWNKZUPGNJKNNX-ZHACJKMWSA-N

Formula: C19H18O4

SMILES: CC(C)=CCOC(=O)C=CC(=O)Oc1cccc2ccccc12

Mol. weight [g/mol]: 310.34

Physical Properties

Property code	Value	Unit	Source
gf	2.58	kJ/mol	Joback Method
hf	-284.31	kJ/mol	Joback Method
hfus	40.30	kJ/mol	Joback Method
hvap	80.77	kJ/mol	Joback Method
log10ws	-5.09		Crippen Method
logp	3.811		Crippen Method
mcvol	241.630	ml/mol	McGowan Method
pc	1923.67	kPa	Joback Method
rinpol	2540.00		NIST Webbook
rinpol	2540.00		NIST Webbook
tb	845.54	K	Joback Method
tc	1075.55	K	Joback Method
tf	495.73	K	Joback Method
vc	0.922	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	691.47	J/mol×K	845.54	Joback Method
cpg	705.03	J/mol×K	883.88	Joback Method
cpg	717.67	J/mol×K	922.21	Joback Method
cpg	729.46	J/mol×K	960.55	Joback Method
cpg	740.50	J/mol×K	998.88	Joback Method
cpg	750.88	J/mol×K	1037.22	Joback Method
cpg	760.68	J/mol×K	1075.55	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405807&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
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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