Fumaric acid, naphth-2-yl hept-2-yl ester

Inchi: InChI=1S/C21H24O4/c1-3-4-5-8-16(2)24-20(22)13-14-21(23)25-19-12-11-17-9-6-7-10-18
InchiKey: PBPKONUILXVONK-BUHFOSPRSA-N
Formula: C21H24O4
SMILES: CCCCCC(C)OC(=O)C=CC(=O)Oc1ccc2ccccc2c1
Mol. weight [g/mol]: 340.41

Physical Properties

Property code	Value	Unit	Source
gf	-54.69	kJ/mol	Joback Method
hf	-438.30	kJ/mol	Joback Method
hfus	43.07	kJ/mol	Joback Method
hvap	84.80	kJ/mol	Joback Method
log10ws	-6.19		Crippen Method
logp	4.813		Crippen Method
mcvol	274.110	ml/mol	McGowan Method
pc	1573.45	kPa	Joback Method
rinpol	2698.00		NIST Webbook
rinpol	2698.00		NIST Webbook
tb	886.82	K	Joback Method
tc	1107.45	K	Joback Method
tf	522.31	K	Joback Method
vc	1.048	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	834.06	J/mol×K	886.82	Joback Method
cpg	848.53	J/mol×K	923.59	Joback Method
cpg	861.97	J/mol×K	960.36	Joback Method
cpg	874.45	J/mol×K	997.13	Joback Method
cpg	886.03	J/mol×K	1033.90	Joback Method
cpg	896.79	J/mol×K	1070.68	Joback Method
cpg	906.81	J/mol×K	1107.45	Joback Method
dvisc	0.0006494	Pa×s	522.31	Joback Method

dvisc	0.0003772	Pa×s	583.06	Joback Method
dvisc	0.0002428	Pa×s	643.81	Joback Method
dvisc	0.0001686	Pa×s	704.56	Joback Method
dvisc	0.0001241	Pa×s	765.32	Joback Method
dvisc	0.0000955	Pa×s	826.07	Joback Method
dvisc	0.0000762	Pa×s	886.82	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=U405829&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