9H-Fluorene-9-carboxylic acid, hexyl ester

Inchi: InChI=1S/C20H22O2/c1-2-3-4-9-14-22-20(21)19-17-12-7-5-10-15(17)16-11-6-8-13-18(16
InchiKey: HOXNWWCBJKARBH-UHFFFAOYSA-N
Formula: C20H22O2
SMILES: CCCCCCOC(=O)C1c2ccccc2-c2ccccc21
Mol. weight [g/mol]: 294.39

Physical Properties

Property code	Value	Unit	Source
gf	174.11	kJ/mol	Joback Method
hf	-165.69	kJ/mol	Joback Method
hfus	39.98	kJ/mol	Joback Method
hvap	74.72	kJ/mol	Joback Method
log10ws	-6.18		Crippen Method
logp	4.922		Crippen Method
mcvol	241.720	ml/mol	McGowan Method
pc	1765.41	kPa	Joback Method
rinpol	3216.00		NIST Webbook
rinpol	3216.00		NIST Webbook
tb	794.81	K	Joback Method
tc	1015.20	K	Joback Method
tf	490.18	K	Joback Method
vc	0.936	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	713.75	J/mol×K	794.81	Joback Method
cpg	784.64	J/mol×K	978.46	Joback Method
cpg	772.07	J/mol×K	941.73	Joback Method
cpg	758.79	J/mol×K	905.00	Joback Method
cpg	744.71	J/mol×K	868.27	Joback Method
cpg	729.73	J/mol×K	831.54	Joback Method
cpg	796.59	J/mol×K	1015.20	Joback Method
dvisc	0.0004567	Pa×s	794.81	Joback Method

dvisc	0.0005232	Pa×s	744.04	Joback Method
dvisc	0.0006114	Pa×s	693.27	Joback Method
dvisc	0.0007324	Pa×s	642.50	Joback Method
dvisc	0.0009049	Pa×s	591.72	Joback Method
dvisc	0.0011633	Pa×s	540.95	Joback Method
dvisc	0.0015753	Pa×s	490.18	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=U415129&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