2-sec-butyl-6-isopropylphenol

Inchi: InChI=1S/C13H20O/c1-5-10(4)12-8-6-7-11(9(2)3)13(12)14/h6-10,14H,5H2,1-4H3
InchiKey: NMTCMJXRNZCLIH-UHFFFAOYSA-N
Formula: C13H20O
SMILES: CCC(C)c1cccc(C(C)C)c1O
Mol. weight [g/mol]: 192.30
CAS: 74926-97-9

Physical Properties

Property code	Value	Unit	Source
af	0.5855		Cheméo Relay (1.0)
hf	-267.02	kJ/mol	Cheméo Relay (1.0)
hfus	21.82	kJ/mol	Joback Method
hvap	86.96	kJ/mol	Cheméo Relay (1.0)
ie	7.93	eV	Cheméo Relay (1.0)
log10ws	-3.69		Cheméo Relay (1.0)
logp	4.029		Crippen Method
mcvol	176.140	ml/mol	McGowan Method
pc	2537.93	kPa	Joback Method
tb	523.10	K	Cheméo Relay (1.0)
tc	752.29	K	Cheméo Relay (1.0)
tf	309.94	K	Cheméo Relay (1.0)
vc	0.619	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	455.12	J/mol×K	608.24	Joback Method
cpg	540.04	J/mol×K	825.55	Joback Method
cpg	527.83	J/mol×K	789.33	Joback Method
cpg	514.95	J/mol×K	753.11	Joback Method
cpg	501.31	J/mol×K	716.89	Joback Method
cpg	486.85	J/mol×K	680.68	Joback Method
cpg	471.48	J/mol×K	644.46	Joback Method
dvisc	0.0001475	Pa×s	482.59	Joback Method

dvisc	0.0000255	Pa×s	608.24	Joback Method
dvisc	0.0000419	Pa×s	566.36	Joback Method
dvisc	0.0000748	Pa×s	524.47	Joback Method
dvisc	0.0029475	Pa×s	356.93	Joback Method
dvisc	0.0003311	Pa×s	440.70	Joback Method
dvisc	0.0008808	Pa×s	398.81	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.43512e+01
Coeff. B	-4.43720e+03
Coeff. C	-8.84900e+01
Temperature range (K), min.	404.00
Temperature range (K), max.	579.35

Sources

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions

hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume