

trans-Acenaphthen-1,2-diol

Inchi:	InChI=1S/C12H10O2/c13-11-8-5-1-3-7-4-2-6-9(10(7)8)12(11)14/h1-6,11-14H/t11-,12-/m1
InchiKey:	ARGFAPRYULRPAN-VXGBXAGGSA-N
Formula:	C12H10O2
SMILES:	OC1c2cccc3cccc(c23)C1O
Mol. weight [g/mol]:	186.21

Physical Properties

Property code	Value	Unit	Source
gf	41.46	kJ/mol	Joback Method
hf	-132.19	kJ/mol	Joback Method
hfus	26.60	kJ/mol	Joback Method
hvap	80.34	kJ/mol	Joback Method
log10ws	-3.38		Crippen Method
logp	1.920		Crippen Method
mcvol	137.600	ml/mol	McGowan Method
pc	4067.32	kPa	Joback Method
rinpol	1830.00		NIST Webbook
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tb	711.74	K	Joback Method
tc	917.91	K	Joback Method
tf	448.02	K	Joback Method
vc	0.523	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	378.85	J/mol×K	711.74	Joback Method
cpg	420.93	J/mol×K	883.55	Joback Method
cpg	413.36	J/mol×K	849.19	Joback Method
cpg	405.44	J/mol×K	814.82	Joback Method
cpg	397.10	J/mol×K	780.46	Joback Method
cpg	388.26	J/mol×K	746.10	Joback Method
cpg	428.22	J/mol×K	917.91	Joback Method
dvisc	0.0001028	Pa×s	711.74	Joback Method

dvisc	0.0001425	Pa×s	667.79	Joback Method
dvisc	0.0002070	Pa×s	623.83	Joback Method
dvisc	0.0003180	Pa×s	579.88	Joback Method
dvisc	0.0005244	Pa×s	535.93	Joback Method
dvisc	0.0009455	Pa×s	491.97	Joback Method
dvisc	0.0019138	Pa×s	448.02	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=R109643&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

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