

(-)-ar-Curcumen-15-al

Other names:	ar-Curcumen-15-al
Inchi:	InChI=1S/C15H20O/c1-12(2)5-4-6-13(3)15-9-7-14(11-16)8-10-15/h5,7-11,13H,4,6H2,1-3
InchiKey:	XVWGGKCJOXAGDW-UHFFFAOYSA-N
Formula:	C15H20O
SMILES:	<chem>CC(C)=CCCC(C)c1ccc(C=O)cc1</chem>
Mol. weight [g/mol]:	216.32

Physical Properties

Property code	Value	Unit	Source
gf	147.91	kJ/mol	Joback Method
hf	-111.30	kJ/mol	Joback Method
hfus	25.92	kJ/mol	Joback Method
hvap	58.29	kJ/mol	Joback Method
log10ws	-4.84		Crippen Method
logp	4.349		Crippen Method
mcvol	195.720	ml/mol	McGowan Method
pc	2060.49	kPa	Joback Method
rinpol	1691.00		NIST Webbook
rinpol	1691.00		NIST Webbook
rinpol	1690.00		NIST Webbook
rinpol	1690.00		NIST Webbook
ripol	2229.00		NIST Webbook
ripol	2229.00		NIST Webbook
tb	626.52	K	Joback Method
tc	837.47	K	Joback Method
tf	305.71	K	Joback Method
vc	0.759	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	497.73	J/molxK	626.52	Joback Method
cpg	514.52	J/molxK	661.68	Joback Method
cpg	530.28	J/molxK	696.84	Joback Method

cpg	545.08	J/mol×K	732.00	Joback Method
cpg	558.98	J/mol×K	767.15	Joback Method
cpg	572.01	J/mol×K	802.31	Joback Method
cpg	584.26	J/mol×K	837.47	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R233419&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/78-624-3/ar-Curcumen-15-al.pdf>

Generated by Cheméo on 2024-04-19 21:00:22.690177683 +0000 UTC m=+15849671.610754998.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.