

trans-Pinocarvyl caprate

Inchi:	InChI=1S/C20H34O2/c1-5-6-7-8-9-10-11-12-19(21)22-18-14-16-13-17(15(18)2)20(16,3)4
InchiKey:	UAQXIEIGKOSXLQ-UHFFFAOYSA-N
Formula:	C20H34O2
SMILES:	<chem>C=C1C(OC(=O)CCCCCCCC)CC2CC1C2(C)C</chem>
Mol. weight [g/mol]:	306.48

Physical Properties

Property code	Value	Unit	Source
gf	25.17	kJ/mol	Joback Method
hf	-502.69	kJ/mol	Joback Method
hfus	39.20	kJ/mol	Joback Method
hvap	67.66	kJ/mol	Joback Method
log10ws	-6.09		Crippen Method
logp	5.661		Crippen Method
mvol	274.080	ml/mol	McGowan Method
pc	1267.35	kPa	Joback Method
rinpol	2093.10		NIST Webbook
rinpol	2093.10		NIST Webbook
tb	741.10	K	Joback Method
tc	932.25	K	Joback Method
tf	448.78	K	Joback Method
vc	1.065	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	856.94	J/mol×K	741.10	Joback Method
cpg	877.71	J/mol×K	772.96	Joback Method
cpg	897.67	J/mol×K	804.82	Joback Method
cpg	916.93	J/mol×K	836.67	Joback Method
cpg	935.60	J/mol×K	868.53	Joback Method
cpg	953.79	J/mol×K	900.39	Joback Method
cpg	971.59	J/mol×K	932.25	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U414146&Units=SI

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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