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: C=C1C(OC(=O)CCCCCCCCC)CC2CC1C2(C)C
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
mcvol	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	m3/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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U414146&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
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/80-609-7/trans-Pinocarvyl-caprate.pdf

Generated by Cheméo on 2024-10-12 09:29:33.054079071 +0000 UTC m=+3306235.691048323.

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