Myrtenyl caprate

Inchi: InChI=1S/C20H34O2/c1-4-5-6-7-8-9-10-11-19(21)22-15-16-12-13-17-14-18(16)20(17,2)3
InchiKey: LQMAKCSAHVRHGY-UHFFFAOYSA-N
Formula: C20H34O2
SMILES: CCCCCCCCCC(=O)OCC1=CCC2CC1C2(C)C
Mol. weight [g/mol]: 306.48

Physical Properties

Property code	Value	Unit	Source
gf	0.13	kJ/mol	Joback Method
hf	-520.28	kJ/mol	Joback Method
hfus	40.12	kJ/mol	Joback Method
hvap	68.76	kJ/mol	Joback Method
log10ws	-5.97		Crippen Method
logp	5.663		Crippen Method
mcvol	274.080	ml/mol	McGowan Method
pc	1299.53	kPa	Joback Method
rinpol	2126.00		NIST Webbook
rinpol	2126.00		NIST Webbook
tb	750.75	K	Joback Method
tc	943.14	K	Joback Method
tf	452.62	K	Joback Method
vc	1.069	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	855.71	J/mol×K	750.75	Joback Method
cpg	875.99	J/mol×K	782.81	Joback Method
cpg	895.52	J/mol×K	814.88	Joback Method
cpg	914.43	J/mol×K	846.94	Joback Method
cpg	932.82	J/mol×K	879.01	Joback Method
cpg	950.81	J/mol×K	911.07	Joback Method
cpg	968.52	J/mol×K	943.14	Joback Method

Sources

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=U414145&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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/87-808-9/Myrtenyl-caprate.pdf
Generated by Cheméo on 2024-04-25 17:05:18.708931506 +0000 UTC m=+16353967.629508826.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.