Brassicasterone

Other names: Brassicasterone
Inchi: InChI=1S/C28H44O/c1-18(2)19(3)7-8-20(4)24-11-12-25-23-10-9-21-17-22(29)13-15-27(2
InchiKey: OWYXOXZSAKVGHJ-BQYQJAHWSA-N
Formula: C28H44O
SMILES: CC(C)C(C)/C=C/C(C)C1CCC2C3CCC4=CC(=O)CCC4(C)C3CCC12C
Mol. weight [g/mol]: 396.66

Physical Properties

Property code	Value	Unit	Source
hfus	29.84	kJ/mol	Joback Method
log10ws	-7.35		Cheméo Relay (1.0)
logp	7.619		Crippen Method
mcvol	354.910	ml/mol	McGowan Method
rinpol	3235.00		NIST Webbook
tf	426.94	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1318.15	J/mol×K	954.29	Joback Method
cpg	1350.90	J/mol×K	994.39	Joback Method
cpg	1384.22	J/mol×K	1034.49	Joback Method
cpg	1418.50	J/mol×K	1074.60	Joback Method
cpg	1454.13	J/mol×K	1114.70	Joback Method
cpg	1491.51	J/mol×K	1154.80	Joback Method
cpg	1531.03	J/mol×K	1194.90	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4030926&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point