

10b,10c-Dihydro-10b,10c-dipropyl-trans-pyrene

Inchi:	InChI=1S/C22H24/c1-3-15-21-17-7-5-8-18(21)12-14-20-10-6-9-19(13-11-17)22(20,21)16
InchiKey:	CNURFFWIKKDBJB-HZCBDIJESA-N
Formula:	C22H24
SMILES:	CCCC12C3=CC=CC1=CC=C1C=CC=C(C=C3)C12CCC
Mol. weight [g/mol]:	288.43

Physical Properties

Property code	Value	Unit	Source
gf	504.60	kJ/mol	Joback Method
hf	198.89	kJ/mol	Joback Method
hfus	29.14	kJ/mol	Joback Method
hvap	67.91	kJ/mol	Joback Method
log10ws	-7.10		Crippen Method
logp	5.988		Crippen Method
mvol	247.300	ml/mol	McGowan Method
pc	1792.42	kPa	Joback Method
rinpol	422.70		NIST Webbook
tb	770.66	K	Joback Method
tc	1009.51	K	Joback Method
tf	507.06	K	Joback Method
vc	0.964	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	728.07	J/mol×K	770.66	Joback Method
cpg	747.97	J/mol×K	810.47	Joback Method
cpg	767.90	J/mol×K	850.28	Joback Method
cpg	788.30	J/mol×K	890.09	Joback Method
cpg	809.58	J/mol×K	929.89	Joback Method
cpg	832.16	J/mol×K	969.70	Joback Method
cpg	856.46	J/mol×K	1009.51	Joback Method

Sources

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=R532439&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	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

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