4-cyanobenzoic acid, 4-hexadecyl ester

Inchi: InChI=1S/C24H37NO2/c1-3-5-6-7-8-9-10-11-12-13-15-23(14-4-2)27-24(26)22-18-16-21(
InchiKey: KEOGVJFULGMUAY-UHFFFAOYSA-N
Formula: C24H37NO2
SMILES: CCCCCCCCCCCCCC(CCC)OC(=O)c1ccc(C#N)cc1
Mol. weight [g/mol]: 371.56

Physical Properties

Property code	Value	Unit	Source
hfus	52.34	kJ/mol	Joback Method
ie	9.67	eV	Cheméo Relay (1.0)
logp	7.195		Crippen Method
mcvol	334.080	ml/mol	McGowan Method
rinpol	2541.00		NIST Webbook
tf	304.15	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1101.58	J/mol×K	958.11	Joback Method
cpg	1117.92	J/mol×K	994.09	Joback Method
cpg	1133.02	J/mol×K	1030.07	Joback Method
cpg	1146.94	J/mol×K	1066.05	Joback Method
cpg	1159.74	J/mol×K	1102.03	Joback Method
cpg	1171.46	J/mol×K	1138.02	Joback Method
cpg	1182.18	J/mol×K	1174.00	Joback Method

Sources

Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U292454&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

Legend

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