

1,2-Cyclohexanedicarboxylic acid, allyl octadecyl ester

Inchi:	InChI=1S/C29H52O4/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-21-25-33-29(31)27-23
InchiKey:	HEFFSOHYOKUWFM-UHFFFAOYSA-N
Formula:	C29H52O4
SMILES:	C=CCOC(=O)C1CCCCC1C(=O)OCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]:	464.72

Physical Properties

Property code	Value	Unit	Source
gf	-169.96	kJ/mol	Joback Method
hf	-972.08	kJ/mol	Joback Method
hfus	68.07	kJ/mol	Joback Method
hvap	97.91	kJ/mol	Joback Method
log10ws	-8.95		Crippen Method
logp	8.327		Crippen Method
mvol	419.190	ml/mol	McGowan Method
pc	732.04	kPa	Joback Method
rinpol	3296.00		NIST Webbook
rinpol	3296.00		NIST Webbook
tb	1027.06	K	Joback Method
tc	1265.00	K	Joback Method
tf	562.29	K	Joback Method
vc	1.621	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1508.93	J/molxK	1027.06	Joback Method
cpg	1590.10	J/molxK	1225.34	Joback Method
cpg	1577.88	J/molxK	1185.69	Joback Method
cpg	1563.73	J/molxK	1146.03	Joback Method
cpg	1547.57	J/molxK	1106.37	Joback Method
cpg	1529.33	J/molxK	1066.72	Joback Method
cpg	1600.47	J/molxK	1265.00	Joback Method
dvisc	0.0000202	Paxs	1027.06	Joback Method

dvisc	0.0000269	Paxs	949.60	Joback Method
dvisc	0.0000376	Paxs	872.14	Joback Method
dvisc	0.0000561	Paxs	794.67	Joback Method
dvisc	0.0000914	Paxs	717.21	Joback Method
dvisc	0.0001675	Paxs	639.75	Joback Method
dvisc	0.0003628	Paxs	562.29	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339494&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
dvisc:	Dynamic viscosity
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

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