

Isovaleric acid, tetracosyl ester

Inchi: InChI=1S/C29H58O2/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25
InchiKey: IDPXGDLRSHZFIZ-UHFFFAOYSA-N
Formula: C29H58O2
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCOC(=O)CC(C)C
Mol. weight [g/mol]: 438.77

Physical Properties

Property code	Value	Unit	Source
gf	-43.06	kJ/mol	Joback Method
hf	-891.97	kJ/mol	Joback Method
hfus	70.13	kJ/mol	Joback Method
hvap	88.92	kJ/mol	Joback Method
log10ws	-10.58		Crippen Method
logp	10.178		Crippen Method
mvol	426.910	ml/mol	McGowan Method
pc	641.57	kPa	Joback Method
rinpol	3043.90		NIST Webbook
rinpol	3043.90		NIST Webbook
tb	938.77	K	Joback Method
tc	1159.48	K	Joback Method
tf	473.75	K	Joback Method
vc	1.677	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1482.71	J/molxK	938.77	Joback Method
cpg	1591.72	J/molxK	1122.69	Joback Method
cpg	1573.05	J/molxK	1085.91	Joback Method
cpg	1552.90	J/molxK	1049.12	Joback Method
cpg	1531.17	J/molxK	1012.34	Joback Method
cpg	1507.81	J/molxK	975.55	Joback Method
cpg	1608.98	J/molxK	1159.48	Joback Method
dvisc	0.0000179	Paxs	938.77	Joback Method

dvisc	0.0000250	Paxs	861.27	Joback Method
dvisc	0.0000371	Paxs	783.76	Joback Method
dvisc	0.0000601	Paxs	706.26	Joback Method
dvisc	0.0001097	Paxs	628.76	Joback Method
dvisc	0.0002372	Paxs	551.25	Joback Method
dvisc	0.0006598	Paxs	473.75	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U414237&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

Latest version available from:

<https://www.chemeo.com/cid/83-050-4/Isovaleric-acid-tetracosyl-ester.pdf>

Generated by Cheméo on 2024-04-19 02:17:32.272654209 +0000 UTC m=+15782301.193231520.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.