

Adipic acid, eicosyl 3-methylpentyl ester

Inchi: InChI=1S/C32H62O4/c1-4-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-24-28-35-31(3)
InchiKey: KUGGRFJUXCDDDBV-UHFFFAOYSA-N
Formula: C32H62O4
SMILES: CCCCCCCCCCCCCCCCCCCCCOC(=O)CCCCC(=O)OCCC(C)CC
Mol. weight [g/mol]: 510.83

Physical Properties

Property code	Value	Unit	Source
gf	-251.72	kJ/mol	Joback Method
hf	-1198.69	kJ/mol	Joback Method
hfus	80.69	kJ/mol	Joback Method
hvap	104.75	kJ/mol	Joback Method
log10ws	-10.70		Crippen Method
logp	10.111		Crippen Method
mvol	476.620	ml/mol	McGowan Method
pc	569.60	kPa	Joback Method
rinpol	3517.00		NIST Webbook
rinpol	3517.00		NIST Webbook
tb	1083.70	K	Joback Method
tc	1379.80	K	Joback Method
tf	579.72	K	Joback Method
vc	1.869	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1736.88	J/molxK	1083.70	Joback Method
cpg	1762.49	J/molxK	1133.05	Joback Method
cpg	1784.99	J/molxK	1182.40	Joback Method
cpg	1804.54	J/molxK	1231.75	Joback Method
cpg	1821.32	J/molxK	1281.10	Joback Method
cpg	1835.51	J/molxK	1330.45	Joback Method
cpg	1847.27	J/molxK	1379.80	Joback Method
dvisc	0.0002008	Paxs	579.72	Joback Method

dvisc	0.0000821	Paxs	663.72	Joback Method
dvisc	0.0000410	Paxs	747.71	Joback Method
dvisc	0.0000236	Paxs	831.71	Joback Method
dvisc	0.0000150	Paxs	915.71	Joback Method
dvisc	0.0000103	Paxs	999.70	Joback Method
dvisc	0.0000075	Paxs	1083.70	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353705&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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