

di-n-Amylfumarate

Other names:	Dipentyl fumarate
Inchi:	InChI=1S/C14H24O4/c1-3-5-7-11-17-13(15)9-10-14(16)18-12-8-6-4-2/h9-10H,3-8,11-12H
InchiKey:	NFCMRHDORQSGIS-MDZDMXLPSA-N
Formula:	C14H24O4
SMILES:	CCCCCOC(=O)C=CC(=O)OCCCCC
Mol. weight [g/mol]:	256.34
CAS:	20314-74-3

Physical Properties

Property code	Value	Unit	Source
gf	-320.62	kJ/mol	Joback Method
hf	-704.67	kJ/mol	Joback Method
hfus	37.79	kJ/mol	Joback Method
hvap	65.03	kJ/mol	Joback Method
log10ws	-3.26		Crippen Method
logp	3.009		Crippen Method
mcvol	218.700	ml/mol	McGowan Method
pc	1710.36	kPa	Joback Method
rinpol	1558.00		NIST Webbook
tb	676.46	K	Joback Method
tc	857.71	K	Joback Method
tf	386.78	K	Joback Method
vc	0.848	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	600.12	J/molxK	676.46	Joback Method
cpg	668.66	J/molxK	827.50	Joback Method
cpg	656.37	J/molxK	797.29	Joback Method
cpg	643.39	J/molxK	767.08	Joback Method
cpg	629.69	J/molxK	736.88	Joback Method
cpg	615.28	J/molxK	706.67	Joback Method
cpg	680.26	J/molxK	857.71	Joback Method

dvisc	0.0001031	Paxs	676.46	Joback Method
dvisc	0.0001345	Paxs	628.18	Joback Method
dvisc	0.0001834	Paxs	579.90	Joback Method
dvisc	0.0002647	Paxs	531.62	Joback Method
dvisc	0.0004109	Paxs	483.34	Joback Method
dvisc	0.0007034	Paxs	435.06	Joback Method
dvisc	0.0013772	Paxs	386.78	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	465.00 ± 1.00	K	3.30	NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20314743&Units=SI

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature

tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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