

Sebacic acid, 4-bromophenyl decyl ester

Inchi:	InChI=1S/C26H41BrO4/c1-2-3-4-5-6-9-12-15-22-30-25(28)16-13-10-7-8-11-14-17-26(29)
InchiKey:	BNYSARVBHXNBML-UHFFFAOYSA-N
Formula:	C26H41BrO4
SMILES:	CCCCCCCCCOC(=O)CCCCCCCC(=O)Oc1ccc(Br)cc1
Mol. weight [g/mol]:	497.50

Physical Properties

Property code	Value	Unit	Source
gf	-182.70	kJ/mol	Joback Method
hf	-818.18	kJ/mol	Joback Method
hfus	67.61	kJ/mol	Joback Method
hvap	101.15	kJ/mol	Joback Method
log10ws	-9.35		Crippen Method
logp	8.159		Crippen Method
mvol	385.820	ml/mol	McGowan Method
pc	954.37	kPa	Joback Method
rinpol	3515.00		NIST Webbook
rinpol	3515.00		NIST Webbook
tb	1044.68	K	Joback Method
tc	1281.15	K	Joback Method
tf	625.84	K	Joback Method
vc	1.494	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1283.30	J/molxK	1044.68	Joback Method
cpg	1299.27	J/molxK	1084.09	Joback Method
cpg	1313.68	J/molxK	1123.50	Joback Method
cpg	1326.62	J/molxK	1162.92	Joback Method
cpg	1338.15	J/molxK	1202.33	Joback Method
cpg	1348.36	J/molxK	1241.74	Joback Method
cpg	1357.32	J/molxK	1281.15	Joback Method
dvisc	0.0001884	Paxs	625.84	Joback Method

dvisc	0.0001030	Paxs	695.65	Joback Method
dvisc	0.0000629	Paxs	765.45	Joback Method
dvisc	0.0000417	Paxs	835.26	Joback Method
dvisc	0.0000295	Paxs	905.07	Joback Method
dvisc	0.0000219	Paxs	974.87	Joback Method
dvisc	0.0000169	Paxs	1044.68	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=U354771&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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